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(54) Title: UNDECAPRENYL PYROPHOSPHATE SYNTHASE (UPPS) ENZYME AND METHODS OF USE

UNDECAPRENYL PYROPHOSPHATE SYNTHASE (UPPS) ENZYME AND METHODS OF USE

Technical Field of the Invention

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The present invention relates generally to the identification of a novel undecaprenyl pyrophosphate synthase (herein "UPPS") crystalline structure. In addition, it provides a novel undecaprenyl pyrophosphate synthase active site of a crystalline structure in complex with Isopentenyl pyrophosphate and in complex with farnesyl pyrophosphate and methods to use these crystalline forms and their active sites to identify and improve undecaprenyl pyrophosphate synthase inhibitor compounds, among other uses. These compounds are characterized by the ability to competitively inhibit binding of substrates or other likemolecules to the active site of UPPS.

Background of the Invention

Polyisoprenoid molecules constitute a diverse and essential group of cellular polymers that function as sugar transporters, pigments, vitamins, hormones, etc. These molecules are products of a condensation of isopentenyl units that are produced by either of two pathways, a mevalonate-dependent or a mevalonate-independent pathway. IPP is a building block in the synthesis of squalene from which steroids are produced, and it is also a precursor of geranyl pyrophosphate from which polyisoprenols are synthesized (C. K. Mathews, and K. E. van Holde, 1996, Biochemistry). The successive condensation reactions to produce polyisoprenols from IPP are catalyzed by prenyltransferases of which there are at least 16 different enzyme forms in four distinct classes. These classes differ in the stereochemistry of the reaction they catalyze, the chain length of the substrates they use, and the chain length of their products. In the proposed two-step general mechanism of prenyltransferases, the first step is the elimination of the diphosphate from the allylic substrate, followed by the attack of the incoming IPP substrate to form a new carbon-carbon bond, followed by a stereospecific removal of a proton and formation of a new double bond (K. Ogura, and T. Koyama (1998) Chemical Reviews 98, 1263-1276; S. Ohnuma, T. Koyama, and K. Ogura (1989) FEBS Letters 257, 71-74).

In one of their many functions throughout the cell, polyisoprenol molecules are used as essential sugar carriers in the biosynthesis of glycoproteins in mammalian cells, and as essential sugar carriers in the biosynthesis of the bacterial cell wall. The peptidoglycan of the bacterial cell wall of Gram positive bacteria is formed by alternating units of N-acetylglucosamine, NAcGlc and N-acetylmuramic acid, NacMur. A pentapeptide chain with

sequence: (L-Ala)-(D-Glu)-(L-Lys)-(D-Ala)-(D-Ala) is linked through the N-terminal amino group of the peptide with the carboxyl group of the lactate moiety of NAcMur. These peptidoglycan chains are further cross-linked by connecting pentaglycine units. The NAcMur-pentapeptide is synthesized from UDP-NAcMur by successive additions of the corresponding amino acids catalyzed by various ligases, after which the NacMurpentapeptide is transferred to undecaprenolphosphate with the release of UMP. While linked to the undecaprenol carrier, NAcGlc and five glycine residues are added from Gly-tRNA. Subsequently, the NacGlc-NacMur-pentapeptide-pentaglycine intermediate is transferred to a peptidoglycan acceptor with the release of undecaprenyl pyrophosphate. In the next step, the terminal D-Ala is cleaved and released as adjacent peptidoglycan chains are cross-linked between the penultimate D-Ala of the first chain and the •-NH group of the lysine in the second chain. It is noteworthy that several molecules with antibacterial activity block various steps along this pathway. For example, bacitracin blocks the hydrolysis of the phosphodiester bond of undacaprenyl pyrophosphate to produce undecaprenylphosphate; vancomycin blocks the transfer of NacGlc-NacMur-pentapeptide-pentaglycine to the acceptor; and penicillin and cephalosporins block the transpeptidation, or cross-linking, between adjacent peptidoglycan chains.

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The sugar-carrier function of undecaprenolphosphate in bacteria is performed in mammalian cells by dolicholphosphate during N-linked glycosylation of peptides in the ER. 20 The human and bacterial homologous enzymes share about 34% amino acid sequence identity. Unlike undecaprenol, formed by 11 isopentenyl units, the dolichol molecule is nearly twice as large with 19-21 units. The amino acid sequence alignment of related UPPSs shows that contrary to other prenyl transferases, UPPS does not have the DDXXD sequence motif (A. Chen, P. A. Kroon, and C. D. Poulter (1994) Protein Science 3, 600-607). Instead, 25 several stretches of highly conserved residues are localized around a shallow cleft on the surface of the protein around the active site. This observation is consistent with the topology observed in the crystal structure of UPPS from Micrococcus luteus B-P 26, (M. Fujihashi, N. Shimizu, Y-W. Zhang, T. Koyama, and K. Miki (1999) Acta Crystallographica D55, 1606-1607; M. Fujihashi, Y-W. Zhang, Y. Higuchi, X-Y. Li, T. Koyama, and K. Miki 30 (2001) Proceedings of the National Academy of Sciences, U.S.A. 98, 4337-4342).

UPP is synthesized by the consecutive action of two enzymes: FPPS and UPPS. The crystal structure of FPPS in complex with FPP shows the FPP molecule bound in a deep pocket at a domain interface with a magnesium ion coordinated between the pyrophosphate and two aspartate residues in the DDXXD motif characteristic of these class of farnesyltransferases (L. C. Tarshis, M. Ynag, C. D. Poulter, and J. C. Sachettini (1994)

Biochemistry 33, 10871-10877). The FPPS product is an (all-E)-farnesyl diphosphate, one of the substrates for UPPS. UPPS is a (Z)-polyprenyldiphosphate synthase (prenyltransferase type IV) that catalyzes the sequential Z-addition of eight IPP molecules to an all-E-FPP to produce a E,Z-mixed-C₅₅-isoprenyldiphosphate product, undecaprenyl pyrophosphate (M. Ito, M. Kobayashi, T. Koyama, and K. Ogura (1987) Biochemistry 26, 4745-4750):

UPPS, detergent,
$$Mg^{2+}$$
(all-E)-FPP + 8 IPP

 $E,Z-C_{55}-PP+8 PP$

The S. pneumoniae UPPS has a FPP K_m of 0.5μM and a PK_m of 3.6μM with a pH optimum of 7.5 - 8.0. The monomer has a pI of 5.1, a Mr • 29,000Da and is physiologically and catalytically active as a dimer. UPPS is an essential enzyme present in both Grampositive and Gram-negative pathogens, except in Mycoplasma (J. D. Mutle, and C. M. Allen (1989) Archives in Biochemistry and Biophysics 230, 49-60; I. Takahashi, and K. Ogura (1982) Journal of Biochemistry 92, 1527-1537; N. Shimizu, T. Kagawa, and K. Ogura (1998) Journal of Biological Chemistry 273, 19476-19481; C. M. Apfel, B. Takaca, M. Fountoulakis, M. Stieger, and W. Keck (1999) Journal of Bacteriology 181, 483-492).

The present invention provides a crystal structure of UPPS from Streptococcus

20 pneumoniae in its native state, and in complex with the substrates FPP and IPP. The

structures show that UPPS is a dimer with an extensive contact area along a dimer interface.

A shallow cleft harbors numerous conserved residues and delimits an active site. Several of
these residues are disordered in a native enzyme but become well ordered in substratebound complexes. The crystal structures of the complexes with each of two substrates, FPP

25 and IPP, provide a detailed description of these substrates' mode of binding, a structure of
the Michaelis complex, certain critical residues involved in binding of substrates. The
bound substrates and the residues that appear responsible for catalysis indicate a reaction
mechanism, and map the available binding pockets used by inhibitors.

30 Summary of the Invention

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In one aspect, the invention provides a composition comprising a UPPS in crystalline form.

In another aspect, the present invention relates to a UPPS protein that is derived from *Streptococcus pneumoniae* comprising the amino acid sequence shown in SEQ ID No. 1 having coordinates of any or all of Tables I-III, said protein in an essentially pure native

form, or a homolog thereof. In a preferred embodiment, the invention provides a UPPS composition wherein said UPPS is a dimer.

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In another aspect, the present invention provides a crystalline form of *Streptococcus* pneumoniae UPPS as derived from models of UPPS comprising coordinates of any or all of Tables I-III.

In yet another aspect, the invention provides a UPPS protein in crystalline form having coordinates of Table IA, and interatomic distances and angles of active site residues listed in Table IIA and/or Table IIIA, respectively, in an essentially pure native form or a homolog thereof.

In yet another aspect, the invention provides a prenyltransferase of a Streptococcus pneumoniae UPPS in its native crystalline form. A preferred embodiment of the invention provides a prenyltransferase wherein said prenyltransferase has an active site formed by the amino acids Arg247, Gly250, Arg206, Arg200, Ser208, Tyr217, Asp28, Tyr70, Ile26, Phe72, Asn76, Met27, Ala71, particularly as ligands to IPP.

In yet another aspect, the invention provides a prenyltransferase wherein said prenyltransferase has an active site formed by the amino acids Asp28-Arg32, Arg79, Met27, His45, Gly48, Met49, Leu52, Ala71, Tyr70, Leu90, Pro91, Phe94, Phe149, particularly as ligands to FPP.

In another aspect, the invention provides a composition comprising a prenyltransferase in complex with FPP as characterized by the coordinates selected from the group consisting of the coordinates of Tables IB, and interatomic distances and angles of active site residues listed in IIB and/or IIIB.

In yet another aspect, the invention provides a composition comprising a prenyltransferase in complex with IPP as characterized by the coordinates selected from the group consisting of the coordinates of Tables IC, and interatomic distances and angles of active site residues listed in IIC and/or IIIC.

In another aspect, the invention provides a heavy atom derivative of a *Streptococcus* pneumoniae UPPS crystal wherein the prenyltransferase comprises a protein having the coordinates represented in any of Figures 2, 3, 4 and/or 5, and listed in Tables IA-IC, IIA-IIC, and/or IIIA-IIIC.

In another aspect, the invention provides a characterized by an $\alpha+\beta$ fold with three layers, $\alpha\beta\alpha$, wherein the β -strands form a six-strand parallel β -sheet and three α -helices pack against one face of the sheet and three to four α -helices located on the opposite face.

In yet another aspect, the invention provides a composition comprising a

Streptococcus pneumoniae UPPS in orthorhombic crystalline form having a space group of

 $P2_12_12_1$ wherin the lattice constants are a = 59.6Å, b = 118.0Å, c = 178.2Å and containing two 60 kDa dimers in an asymmetric unit.

In another aspect, the invention provides a composition comprising a *Streptococcus* pneumoniae UPPS in orthorhombic crystalline form having a space group of I2₁2₁2₁.

In yet another aspect, the invention provides a composition comprising a co-crystal of *Streptococcus pneumoniae* UPPS in complex with IPP in orthorhombic crystalline form having a space group selected from the group consisting of P2₁2₁2₁ and I2₁2₁2.

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In yet another aspect, the invention provides a composition comprising a co-crystal of *Streptococcus pneumoniae* UPPS in complex with a substrate FPP in monoclinic crystalline form having a space group of P2₁ and the crystalline form has lattice constants of a = 58.1 Å, b = 44.6 Å, c = 115.5 Å, $\beta = 98.7^{\circ}$.

In another aspect, the invention provides a process for determining a crystal structure form using structural coordinates of a *Streptococcus pneumoniae* UPPS crystal or portions thereof, to determine a crystal form of a mutant, homologue, or co-complex of said active site by molecular replacement.

In yet another aspect, the invention provides a process of identifying an inhibitor compound capable of binding to and inhibiting an enzymatic activity of a *Streptococcus pneumoniae* UPPS said process comprising: introducing into a suitable computer program information defining an active site conformation of a UPPS molecule comprising a conformation defined by coordinates listed in Table IA, IIA, and/or IIIA wherein said program displays the three-dimensional structure thereof; creating a three dimensional structure of a test compound in said computer program; displaying and superimposing a model of said test compound on a model of said active site; incorporating said test compound in a biological prenyltransferase activity assay for a prenyltransferase characterized by said active site; and determining whether said test compound inhibits enzymatic activity in said assay.

In another aspect, the invention provides a process designing drugs useful for inhibiting UPPS activity using certain or all of the atomic coordinates of a *Streptococcus pneumoniae* UPPS crystal to computationally evaluate a chemical entity for associating with an active site of a UPPS enzyme.

In yet another aspect, the invention provides a method of modifying a test UPPS polypeptide comprising: providing a test UPPS polypeptide sequence having a characteristic that is targeted for modification; aligning the test UPPS polypeptide sequence with at least one reference UPPS polypeptide sequence for which an X-ray structure or other structure is available, wherein the at least one reference UPPS polypeptide sequence has a characteristic

that is desired for the test UPPS polypeptide; building a three-dimensional model for the test UPPS polypeptide using the three-dimensional coordinates of the X-ray structure(s) or other structure(s) of the at least one reference UPPS polypeptide and its sequence alignment with the test UPPS polypeptide sequence; examining the three-dimensional model of the test UPPS polypeptide for a difference in an amino acid residue as compared to the at least one reference polypeptide, wherein the residues are associated with the desired characteristic; and mutating an amino acid residue in the test UPPS polypeptide sequence located at a difference identified to a residue associated with the desired characteristic, whereby the test UPPS polypeptide is modified.

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In another aspect, the invention provides a process of identifying an inhibitor compound capable of inhibiting an enzymatic activity of a *Streptococcus pneumoniae*UPPS, said process comprising: carrying out an *in vitro* assay by introducing said compound in a biological prenyltransferase activity assay containing a prenyltransferase of the invention; and determining whether said test compound inhibits an enzymatic activity of the prenyltransferase in said assay.

In yet another aspect, the invention provides a product of the process of identifying an inhibitor compound capable of inhibiting an enzymatic activity of a *Streptococcus* pneumoniae UPPS which is a peptide, peptidomimetic, or synthetic molecule and is useful for inhibiting the metallo-beta lactamase, preferably in the treatment of bacterial infections in a mammal.

In another aspect, the invention provides a product of the process of identifying an inhibitor compound capable of inhibiting an enzymatic activity of a *Streptococcus* pneumoniae UPPS wherein said product is a competitive or non-competitive inhibitor of the *Streptococcus* pneumoniae prenyltransferase.

In another aspect, the invention provides a process of designing drugs useful for inhibiting Streptococcus pneumoniae UPPS comprising using atomic coordinates of a Streptococcus pneumoniae UPPS crystal or atomic coordinates of a Streptococcus pneumoniae UPPS in complex with FPP or IPP to computationally evaluate a chemical entity for associating with an active site of a Streptococcus pneumoniae UPPS.

In another aspect, the invention provides a process of designing drugs useful for inhibiting Streptococcus pneumoniae UPPS comprising the step of using structure coordinates of Streptococcus pneumoniae UPPS to identify an intermediate in a chemical reaction between said prenyltransferase and a compound that is a substrate or inhibitor of said prenyltransferase. In another aspect, the invention provides a process of designing drugs useful for inhibiting Streptococcus pneumoniae UPPS wherein structure coordinates

comprise the coordinates corresponding to any of the structures shown in Figures 2, 3, 4 and/or 5 and/or listed in Tables IA-IC, IIA-IIC, and/or IIIA-IIIC.

In one aspect, the present invention relates to an UPPS that is derived from Streptococcus pneumoniae and comprising a protein having the amino acid sequence shown in SEQ ID No. 1, and coordinates of Table I, and interatomic distances and angles of active site residues listed in Table II and/or III, in an essentially pure native form or a homolog thereof.

In another aspect, the present invention provides a novel crystalline form of a UPPS enzyme active site in complex with IPP, having the coordinates of Table I, and interatomic distances and angles of active site residues listed in Table II, and/or III.

In yet another aspect, the present invention provides a novel crystalline form of the UPPS enzyme active site in complex with the substrate farnesyl pyrophosphate, identified herein FPP, having the coordinates of Table I, and interatomic distances and angles of active site residues listed in Table II, and/or III.

In yet another aspect, the invention provides a model of specific roles of residues in the active site responsible for the binding of substrates, substrate analogs, and inhibitors.

In yet another aspect, the invention provides astructural basis for the role of active site amino acid residues and metals bound in an active site in a catalytic activity of these enzymes. This aspect of the invention provides a method for identifying inhibitors of a UPPS, which methods comprise the steps of: providing coordinates of a UPP structure of the invention to a computerized modeling system; identifying compounds that bind to an active site; and screening the compounds identified for undecaprenyl pyrophosphate synthase inhibitory bio-activity.

Another aspect of this invention includes machine-readable media encoded with data representing coordinates of a three-dimensional structure of a UPPS crystal structure alone or in complex with IPP and/or FPP.

Other aspects and advantages of the present invention are described further in the following detailed description of the preferred embodiments thereof.

30 <u>Description of the Figures:</u>

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Figure 1A provides a representation of the chemical structure of FPP, and the numbering scheme used.

Figure 1B provides a representation of the chemical structure of IPP, and the numbering scheme used.

Figure 2A provides a representation of the secondary structure elements of native UPPS, from *Streptococcus pneumoniae*.

Figure 2B provides a representation of the topology of UPPS. Triangles denote β -strands and circles denote α -helices.

Figure 3A provides a schematic drawing of a UPPS enzyme from *Streptococcus* pneumoniae in complex with IPP bound in the active site.

Figure 3B provides a schematic drawing of a UPPS enzyme from *Streptococcus* pneumoniae in complex with FPP bound in the active site.

Figure 4A provides a schematic drawing of FPP bound in an active site of UPPS from S. pneumoniae. Shown and labeled in this view are the hydrophobic side chains of residues lining an FPP binding pocket, the interactions of the phosphate groups bound at the N-terminus of $\alpha 1$, a tightly bound water molecule, and the role of conserved arginine residues that are important for FPP binding.

Figure 4B provide a schematic drawing of FPP bound in the active site of UPPS from *S. pneumoniae*. In this view are shown, along the axis of the extended FPP molecule, the relative orientation of the important residues for catalysis, and those side chains important for substrate binding.

Figure 5 provides a schematic drawing of the interactions between the active site residues of a UPPS from *Streptococcus pneumoniae* and the substrate IPP. Important for the substrate binding are arginine side chains from the C-terminus of the other molecule in a dimer. Also shown is a pyrophosphate molecule that occupies the same position as the pyrophosphate moiety of FPP.

Detailed Description of the Invention

The present invention provides a *Streptococcus pneumoniae* UPPS crystalline structure of a native enzyme. In addition, it provides an undecaprenyl pyrophosphate synthase active site of the crystalline structure of the UPPS, in complex with IPP and in complex with FPP and methods to use these crystalline forms and their active sites to identify and improve UPPS inhibitor compounds (peptide, peptidomimetic or synthetic compositions). These compounds are characterized by an ability to competitively inhibit binding of substrates or other like-molecules to the active site of undecaprenyl pyrophosphate synthases.

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A UPPS from Streptococcus pneumoniae crystalline three-dimensional structure and its complex with IPP and FPP

The crystal structures of aUPPS from *Streptococcus pneumoniae* in its native form, in complex with the substrate IPP (Figure 1B), and a substrate, FPP (Figure 1A) have been determined and refined to 2.3Å, 2.8Å and 3.3Å resolution, respectively.

Native UPPS from Streptococcus pneumoniae crystalline structure was determined. This crystal structure consists of two homodimers in the asymmetric unit, molecules A and B form one active dimer, and molecules C and D form the second dimer. A preferred model includes residues 17-72 and 77-248 in molecule A; residues 17-72 and 79-246 in molecule B; residues 17-73 and 77-248 in molecule C; residues 18-73 and 78-246 in molecule D; and a total of 410 water molecules (Figure 2A). Each polypeptide chain has an • + • fold characterized by three layers: • • •. Four •-helices packed against one face of the central •sheet, formed by six parallel •-strands with ordering 342156. Another three •-helices located at the other side of the sheet form most of the dimer interface (Figure 2B). The central sheet is not continuous from one molecule to the other in the dimer, rather, the •sheets from each monomer form an angle of approximately 90°. In the dimer, the N- and the C-terminus of molecule B are located near a shallow groove formed in molecule A, the proposed location of the active site suggesting that the termini on one molecule contribute to the binding of substrates in the other molecule. This may explain the need for the enzyme to be a dimer if catalysis is to occur, and the extensive 1,650 Å² of buried surface area at the dimer interface involving $\alpha 5$, $\alpha 6$, and $\alpha 7$. The dimer interface include interactions between three pairs of charged side chains: Arg170NH2:Asp214OD2 (3.1Å), Arg226NE:Glu239OE2 (2.8Å), and Glu239OE2:Arg226NE (2.6Å). Also across the interface interact Tyr237OH and Asn229ND2 (3.1Å).

There are three buried charged residues: Glu152, Arg200, His22. E152 is at the N-terminus of α 5 and contacts Wat146 (2.9Å), Tyr147OH (2.6Å), Gln214OE1 (3.2Å), Phe184N (2.8Å), and Gln214OE1 (3.1Å). Arg200 is located at the C-terminus of β 5 contacting with Ser218 OG (2.7Å), Arg216O (2.9Å), Asp46OD2 (3.1Å), and Wat410 (2.8Å). His22 is makes H-bonds with Leu192O (2.6Å) and Thr68OG1 (2.9Å).

There are five relatively small, and empty internal cavities. One cavity is next to Arg200, a residue presumably located in the active site. This cavity is bound by atoms in residues Ile198, Ile199, Arg200, Leu20, Leu22, Tyr221 and Phe222. Two more cavities are located on either side of a-helix α3, one is lined by Leu90, Pro91, Phe94, Tyr95, Val99,

Ile109, Ala125, Leu126, Ala129, and Phe143. The cavity on the other side of $\alpha 3$ is lined by His45, Phe86, Met49, Leu90, Leu52, Asn30, Ala71, Met27, and Trp227. The presence of these two cavities suggests that the helix may be displaced upon substrate binding and for product release or membrane association. Another cavity is located C-terminal to $\alpha 6$ and a portion of $\beta 3$ (His187, Phe184, Glu110, Ile112, Asn142, Met111) along the groove on the side of $\alpha 5$. This groove probably accommodates the product. N-terminal to $\beta 5$ is the last cavity (Asp191, Leu192, Arg193, Asp194, Pro195, Asp196) that may allow the $\alpha 6$ - $\beta 5$ connection slide sideways or back and forth when the product is being processed during catalysis. No solvent molecules have been found occupying these cavities.

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In all four molecules in the asymmetric unit, residues 74-76 are disordered in a S. pneumoniae native UPPS structure, and residues in the immediate vicinity have higher B-factors than the average of the structure suggesting that these residues are highly mobile in the absence of ligands or substrates, and that they may be part of the active site. In addition, based on the alignment of UPPS amino acid sequences, the most conserved residues are located in the short α -helix α 1 (residues 28-32) and α 2- β 3 (residues 73-83), and in the β 5- α 7 (residues 200-214) loops suggesting that the active site is located at the top of the sheet in a shallow groove, next to the disordered region. As discussed below, the crystal structures of the UPPS complexes with the substrates FPP and IPP confirm the location of the active site, the critical role played by the conserved residues for substrate binding and their role in catalysis, and show that the disordered residues become ordered upon substrate binding.

The undecaprenyl pyrophosphate synthases from S. pneumoniae and M. luteus share a 37% amino acid sequence identity and the polypeptide have the same fold. Superposition of the $C\alpha$ atoms of the M. luteus and S. pneumoniae native UPPS crystal structures results in an overall root mean square, rms, deviation of 0.6\AA .

The present invention also provides a novel undecaprenyl pyrophosphate synthase crystalline structure based on the UPPS *Streptococcus pneumoniae* undecaprenyl pyrophosphate synthase in complex with the substrates IPP and FPP.

In the FPP complex, one FPP molecule is bound in the active site. However, in the IPP complex structure, two large, adjacent electron density peaks appear in the active site, the first one corresponds to a pyrophosphate onto which the pyrophosphate of FPP can be superimposed. The second electron density peak corresponds to an entire IPP molecule. In both complex structures, the major structural changes between the native and the substrate complex structures is the ordering of the polypeptide chain between residues 72-79, to form two turns of a 3₁₀ helix and the opening of the entrance to the long, narrow hydrophobic

pocket where FPP binds. In the IPP complex, the C-terminus of the other molecule in the dimer also becomes ordered to form part of the IPP binding site.

The interactions between the substrates and the enzyme are summarize as follows:

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- 1. There are at least two substrate-binding sites, at least one of each corresponding to each of the two substrates. The FPP's pyrophosphate binds at the N-terminus of •-helix •1 and the C-terminal end of strands •1 and •2. The farnesyl carbon chain runs across •2 and •3. The IPP's pyrophosphate binding site is located next to an FPP site and also runs across the top strands •1 and •2, but on the other side of the •-sheet. The phosphate group interacts with Arg247 located on the C-terminus of the partner molecule in the dimer
- 2. The farnesyl chain binds into a tunnel lined by Met49, Leu52, Ala71, Leu90, Pro91, Phe94, Leu126, Phe143, and Leu145.
- 3. The isopentenyl chain binds into a shallow depression lined by Ile26, the C• carbon of Asp28, Tyr70, and Phe72. The isopentenyl chain is then substantially or completely enclosed by the farnesyl chain bound adjacent to it and by the C-terminus of the partner molecule in the dimer. They are bound in such a way that the *re* face of an attacking carbon is poised for the reaction.
- 4. The position of the Mg⁺² ions in a metal binding site may be indicated by a strong difference in an electron density peak modeled as a water molecule is located between the two pyrophosphate groups observed bound in the IPP complex.
- 5. The enzymatic turnover cycle starts with binding of FPP required for a subsequent binding of IPP. IPP binding must follow FPP because a binding interaction is with magnesium that is bridging the two pyrophosphates. Also, the carbon chain of FPP forms part of the IPP binding pocket. The orientation of C02 of IPP is such, that C1 of FPP is facing the *re* face of the double bond, ideal for the attack on C1. This is necessary, since the removal of a proton by Asp28 (or Arg200) occurs from the opposite side (on C9) to produce a Z-double bond.
 - 6. A preferred mechanism provides a critical role for His45, in •2, to promote cleavage of the pyrophosphate moiety from FPP by positioning the NE2 atom to polarize C1 in FPP, in analogy to a mechanism of thiamine phosphate synthase. Another preferred mechanism involves a metal-triggered carbocation formation. Once an FPP is bound, the binding of IPP and Mg+2 result in the formation of a carbocation analogously to a mechanism postulated for other prenyltransferases (i.e., farnesyl synthase, or aristolochene synthase). In addition to His45, Asn30 and/or Asp28, or Arg200 in •1 is putatively important for a stereochemically- specific removal of a proton to form a double bond. These residues occupy suitable relative positions for catalysis as deduced from a comparison of

complex structures. Asn30, Asp28 or Arg200 are poised to assist a stereochemical-specific proton abstraction from an incoming isopentenyl unit from C09. These residues are highly conserved among UPPSs from a variety of organisms. Of 27 aligned amino acid sequences including bacterial, archaebacteria and eukariotic UPPS's, the stretch FGHKA that includes Gly44 is absolutely conserved while His45 is present in all but two known sequences. In these two known sequences, a tyrosine replaces the histidine. In the same alignment, an amino acid stretch that includes Asp28, IMDGN, Asp28, Gly29 and Asn30 is absolutely conserved. Site-directed mutagenesis of some conserved residues of UPPS from E. coli (Pan, J-J., Yang, L.-W., and Liang, P-H. (2000) Biochemistry 39, 13856-13861) can now be rationally explained by the discoveries of the present invention. Mutation of Asp26 or Glu213 to alanine causes a 1000-fold drop in k_{cat}. In S. pneumoniae Asp28 is equivalent to E. coli's Asp26. In a preferred catalytic mechanism provided by the invention, Asp28/Asp26 plays a key role in formation of a double bond in the product after condensation step has occurred by removing a proton that would result in a cis (Z) configuration. A second important mutation involves Glu213, in S. pneumoniae Glu219 is equivalent to E. coli's Glu213. Glu219/Glu213 interacts with and helps to position Arg206 in aproper orientation to interact with IPP in an active site. Arg206 is an important residue for binding of IPP.

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Certain mechanisms of the invention take into account the binding of the product's chain when the product exceeds 20 carbons. A model of a C30 intermediate having the preferred stereochemistry (trans, trans, cis, cis, cis) bound at the FPP binding site in an active site UPPS shows that the chain beyond the first 15 carbon atoms can exit the protein into the solvent or, more likely, into a phospholipid membrane or detergent micell through a opening created between helices •2 and •3. Creation of an opening requires the movement of side chains of Met49 and Tyr98, torsion of the side chains is sufficient to open a channel through which a product may exit. There is also the possibility, as has been suggested, that a product may fold on itself several times inside an FPP binding channel, but there does not seem possible since there is not enough space to accommodate a long carbon chain. The final product exits the protein by either a "pull" action from the pyrophosphate end, or by a "pull" action from the opposite end, but that implies that the pyrophosphate is dragged along an FPP binding channel and out through an inter-helix space.

Table I provides the atomic coordinates of preferrednative and complex crystal structures of UPPS from *S. pneumoniae*. This preferred native model includes residues 37-92 and 97-268 in molecule A, 37-92 and 99-266 in molecule B, 37-93 and 97-268 in molecule C, 38-93 and 98-266 in molecule D, for the four molecules, A, B, C, and D, in the crystallographic asymmetric unit. The amino acid sequence of a UPPS from *S. pneumoniae*

is provided in SEQ ID No. 1. Table II provides the distances, in Å, between atoms within a 5.0Å radius in anactive site including bound substrates FPP and IPP. Table III provides the angles (°) between active site atoms at are within 4.0Å of substrate FPP or IPP.

Small variations in the atomic coordinates shown in Tables I - III will occur such as upon refinement of a crystal structure from a different crystal form that will result in a new set of coordinates. The deviation on Cα atoms from the present coordinate set is not expected to substantially exceed a rms of 2.5Å. Similarly, bond angles and bond lengths will usually vary within a small range (Engh, R. A., and Huber, R. (1991) *Acta Crystallogr. A47*, 392-400), however, the inter-atomic interactions in Tables I - III will remain constant, within the experimental error, as will the relative conformation and orientation or positioning of residues in an active site. The atomic coordinates of an active site residues, including bound substrates, are provided in Tables I-III.

Mutants and Derivatives

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Herein, the terms "a" and "an" mean "one or more" when used in this application, including the claims.

The invention further provides homologues, co-complexes, mutants and derivatives of the UPPS crystal structure of the invention.

The term "homologue" means a protein having at least 30% amino acid sequence identity with a functional domain of UPPS. Preferably the percentage identity will be 40, or 50%, more preferably 60 or 70% and most preferably 80 or 90%. A 95% identity is most particularly preferred.

The term "co-complex" means a UPPS or a mutant or homologue of a UPPS in covalent or non-covalent association with a chemical entity or compound.

As used herein, the term "agonist" means an agent that supplements or potentiates the bioactivity of a functional UPPS gene or protein or of a polypeptide encoded by a gene that is up- or down-regulated by a UPPS polypeptide. By way of specific example, an "agonist" is a compound that interacts with a steroid hormone receptor to promote a transcriptional response. An agonist can induce changes in a receptor that places a receptor in an active conformation that allows them to influence transcription, either positively or negatively. There can be several different ligand-induced changes in a receptor's conformation. The term "agonist" specifically encompasses partial agonists.

As used herein, the terms "•-helix", "alpha-helix" and "alpha helix" are used interchangeably and mean the conformation of a polypeptide chain wherein the polypeptide backbone is wound around the long axis of the molecule in a left-handed or right-handed

direction, and the R groups of the amino acids protrude outward from the helical backbone, wherein the repeating unit of the structure is a single turnoff the helix, which extends about 0.56 nm along the long axis.

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As used herein, the term "antagonist" means an agent that decreases or inhibits a bioactivity of a functional UPPS gene or protein, or that supplements or potentiates a bioactivity of a naturally occurring or engineered non-functional UPPS gene or protein. Alternatively, an antagonist can decrease or inhibit a bioactivity of a functional gene or polypeptide encoded by a gene that is up- or down-regulated by a UPPS polypeptide. An antagonist can also supplement or potentiate the bioactivity of a naturally occurring or engineered non-functional gene or polypeptide encoded by a gene that is up- or down-regulated by a UPPS polypeptide. By way of specific example, an "antagonist" is a compound that interacts with a steroid hormone receptor to inhibit a transcriptional response. An antagonist can bind to a receptor but fail to induce conformational changes that alter a receptor's transcriptional regulatory properties or physiologically relevant conformations. Binding of an antagonist can also block the binding and therefore the actions of an agonist. The term "antagonist" specifically encompasses partial antagonists.

As used herein, the terms "•-sheet", "beta-sheet" and "beta sheet" are used interchangeably and mean the conformation of a polypeptide chain stretched into an extended zig-zig conformation. Portions of polypeptide chains that run "parallel" all run in the same direction. Polypeptide chains that are "antiparallel" run in the opposite direction from the parallel chains.

As used herein, the term "binding pocket" refers to any moiety, part or region of UPPS that actually or is capable of binding to, directly participating with, adhering to, or otherwise associating with an atom, ion or molecule. Preferably, a large cavity within a UPPS ligand binding domain where an agonist or antagonist can bind is a binding pocket. Such a cavity can be empty, or can contain water molecules or other molecules from the solvent, or an agonist or antagonist moieties, atoms or molecules. Such a binding pocket also includes regions of space near the "main" binding pocket that are not occupied by atoms or moieties of UPPS, but that are near the "main" binding pocket, and that are contiguous with the "main" binding pocket. Preferably,

As used herein, the term "active site" refers to a specific region of UPPS binding pocket where a molecule binds and catalysis takes place. It is comprised and bound by amino acid residues that are in direct contact with the substrate or that interact with the substrate(s) through water molecules or those amino acids that, although not being in direct contact with the substarte(s), nonetheless are important for they allow the correct

positioning of those amino acids that are and which without the correct positioning they would not be able to interact favorably (i. e. in a way conducent to catalysis) with the substrate(s). These interactions between amino acids and substrate(s) are responsible for the binding of the substrate to UPPS, for the correct positioning of the substrate for catalysis, and for stabilization of any reaction intermediates and for the binding and possibly the release of the products from that active site. These are amino acids that may be replaced by site-directed mutagenesis, and their replacement will result in at the very least a severalfold, or more likely, in several orders of magnitude decrease in the binding affinity of the substrate(s). The active site is also comprised by amino acids that are directly responsible for catalysis. These amino acids interact with the substrate(s) through hydrogen bonds or are in close proximity to electron-donor or electron-acceptor centers in the substrate. These amino acids may act themselves as electron-donor or electron-acceptor centers for catalysis to take place. These are amino acids that may be replaced by site-directed mutagenesis, and their replacement will result in at the very least a several-fold, or more likely, in several orders of magnitude decrease in the catalytic efficiency, but no changes in the affinity of binding of the substarte(s). In some cases, the catalytic activity may be recovered by some chemicals that, by binding to the appropriate active site residues, will mimic the wild-type amino acid.

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As used herein, the term "biological activity" means any observable effect flowing from interaction between a UPPS polypeptide and an agonist or antagonist. Representative, but non-limiting, examples of biological activity in the context of the present invention include transcription regulation, agonist or antagonist binding, and peptide binding.

As used herein, the terms "candidate substance" and "candidate compound" are used interchangeably and refer to a substance that is believed to interact with another moiety, for example an agonist or antagonist that is believed to interact with a complete, or a fragment of, a UPPS polypeptide, and which can be subsequently evaluated for such an interaction. Representative candidate substances or compounds include xenobiotics such as drugs and other therapeutic agents, carcinogens and environmental pollutants, natural products and extracts, as well as endobiotics such as glucocorticosteroids, steroids, fatty acids and prostaglandins. Other examples of candidate compounds that can be investigated using the methods of the present invention include, but are not restricted to, agonists and antagonists of a UPPS polypeptide, toxins and venoms, viral epitopes, hormones (e.g., glucocorticosteroids, opioid peptides, steroids, etc.), hormone receptors, peptides, enzymes, enzyme substrates, co-factors, lectins, sugars, oligonucleotides or nucleic acids, oligosaccharides, proteins, small molecules and monoclonal antibodies.

As used herein, the terms "cells," "host cells" or "recombinant host cells" are used interchangeably and mean not only to a particular subject cell, but also to any progeny or potential progeny of such a cell. Because certain modifications can occur in succeeding generations due to either mutation or environmental influences, such progeny might not, in fact, be identical to the parent cell, but are still included within the scope of the term as used herein.

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As used herein, the terms "chimeric protein" or "fusion protein" are used interchangeably and mean a fusion of a first amino acid sequence encoding a UPPS polypeptide with a second amino acid sequence defining a polypeptide domain foreign to, and not homologous with, any domain of a UPPS polypeptide. A chimeric protein can include a foreign domain that is found in an organism that also expresses the first protein, or it can be an "interspecies" or "intergenic" fusion of protein structures expressed by different kinds of organisms. In general, a fusion protein can be represented by the general formula X—UPPS—Y, wherein UPPS represents a portion of the protein which is derived from a UPPS polypeptide, and X and Y are independently absent or represent amino acid sequences which are not related to a UPPS sequence in an organism, which includes naturally occurring mutants.

As used herein, the term "detecting" means confirming the presence of a target entity by observing the occurrence of a detectable signal, such as a radiologic or spectroscopic signal that will appear exclusively in the presence of the target entity.

As used herein, the term "DNA segment" means a DNA molecule that has been isolated free of total genomic DNA of a particular species. In a preferred embodiment, a DNA segment encoding a UPPS polypeptide refers to a DNA segment that comprises any of SEQ ID NO:1, but can optionally comprise fewer or additional nucleic acids, yet is isolated away from, or purified free from, total genomic DNA of a source species, such as *Streptococcus pnuemoniae*. Included within the term "DNA segment" are DNA segments and smaller fragments of such segments, and also recombinant vectors, including, for example, plasmids, cosmids, phages, viruses, and the like.

As used herein, the term "DNA sequence encoding a UPPS polypeptide" can refer to one or more coding sequences within a particular individual. Moreover, certain differences in nucleotide sequences can exist between individual organisms, which are called alleles. It is possible that such allelic differences might or might not result in differences in amino acid sequence of the encoded polypeptide yet still encode a protein with the same biological activity. As is well known, genes for a particular polypeptide can exist in single or multiple copies within the genome of an individual. Such duplicate genes

can be identical or can have certain modifications, including nucleotide substitutions, additions or deletions, all of which still code for polypeptides having substantially the same activity.

As used herein, the term "expression" generally refers to the cellular processes by which a biologically active polypeptide is produced.

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As used herein, the term "gene" is used for simplicity to refer to a functional protein, polypeptide or peptide encoding unit. As will be understood by those in the art, this functional term includes both genomic sequences and cDNA sequences. Preferred embodiments of genomic and cDNA sequences are disclosed herein.

As used herein, the term "crystal lattice" means the array of points defined by the vertices of packed unit cells.

As used herein, "hexagonal unit cell" means a unit cell wherein $a = b \cdot c$; and $\cdot = \cdot 0$ = 90, $\cdot = 120^{\circ}$. The vectors a, b, and c describe the unit cell edges and the angles \cdot , \cdot , and \cdot describe the unit cell angles. In a preferred embodiment of the present invention, the unit cell has lattice constants of a = 59.6Å, b = 118.0Å, c = 178.2Å. While preferred lattice constants are provided, a crystalline polypeptide of the present invention also comprises variations from the preferred lattice constants, wherein the variations range from about one to about two percent.

As used herein, the term "hybridization" means the binding of a probe molecule, a molecule to which a detectable moiety has been bound, to a target sample.

As used herein, the term "interact" means detectable interactions between molecules, such as can be detected using, for example, a yeast two hybrid assay. The term "interact" is also meant to include "binding" interactions between molecules. Interactions can, for example, be protein-protein or protein-nucleic acid in nature.

As used herein, the term "isolated" means oligonucleotides substantially free of other nucleic acids, proteins, lipids, carbohydrates or other materials with which they can be associated, such association being either in cellular material or in a synthesis medium. The term can also be applied to polypeptides, in which case the polypeptide will be substantially free of nucleic acids, carbohydrates, lipids and other undesired polypeptides.

As used herein, the term "labeled" means the attachment of a moiety, capable of detection by spectroscopic, radiologic or other methods, to a probe molecule.

As used herein, the term "modified" means an alteration from an entity's normally occurring state. An entity can be modified by removing discrete chemical units or by adding discrete chemical units. The term "modified" encompasses detectable labels as well as those entities added as aids in purification.

As used herein, the term "modulate" means an increase, decrease, or other alteration of any or all chemical and biological activities or properties of a wild-type or mutant UPPS polypeptide, preferably a wild-type or mutant UPPS polypeptide. The term "modulation" as used herein refers to both up-regulation (i.e., activation or stimulation) and down-regulation (i.e. inhibition or suppression) of a response, and includes responses that are upregulated in one cell type or tissue, and down-regulated in another cell type or tissue.

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As used herein, the term "molecular replacement" means a method that involves generating a preliminary model of a wild-type UPPS ligand binding domain, or a UPPS mutant crystal whose structure coordinates are unknown, by orienting and positioning a molecule or model whose structure coordinates are known within the unit cell of the unknown crystal so as best to account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This, in turn, can be subject to any of the several forms of refinement to provide a final, accurate structure of the unknown crystal. See, e.g., Lattman, (1985) Method Enzymol., 115: 55-77; Rossmann, ed, (1972) The Molecular Replacement Method, Gordon & Breach, New York. Using the structure coordinates of the active site of UPPS provided by this invention, molecular replacement can be used to determine the structure coordinates of a crystalline mutant or homologue of the UPPS active site, or of a different crystal form of the UPPS active site.

As used herein, the term "partial agonist" means an entity that can bind to a receptor and induce only part of the changes in the receptors that are induced by agonists. The differences can be qualitative or quantitative. Thus, a partial agonist can induce some of the conformation changes induced by agonists, but not others, or it can only induce certain changes to a limited extent.

As used herein, the term "partial antagonist" means an entity that can bind to a receptor and inhibit only part of the changes in the receptors that are induced by antagonists. The differences can be qualitative or quantitative. Thus, a partial antagonist can inhibit some of the conformation changes induced by an antagonist, but not others, or it can inhibit certain changes to a limited extent.

As used herein, the term "polypeptide" means any polymer comprising any of the 20 protein amino acids, regardless of its size. Although "protein" is often used in reference to relatively large polypeptides, and "peptide" is often used in reference to small polypeptides, usage of these terms in the art overlaps and varies. The term "polypeptide" as used herein refers to peptides, polypeptides and proteins, unless otherwise noted. As used

herein, the terms "protein", "polypeptide" and "peptide" are used interchangeably herein when referring to a gene product.

As used herein, the term "primer" means a sequence comprising two or more deoxyribonucleotides or ribonucleotides, preferably more than three, and more preferably more than eight and most preferably at least about 20 nucleotides of an exonic or intronic region. Such oligonucleotides are preferably between ten and thirty bases in length.

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As used herein, the term "sequencing" means the determining the ordered linear sequence of nucleic acids or amino acids of a DNA or protein target sample, using conventional manual or automated laboratory techniques.

As used herein, the terms "structure coordinates" and "structural coordinates" mean mathematical coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a molecule in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal.

Those of skill in the art understand that a set of coordinates determined by X-ray crystallography is not without standard error. In general, the error in the coordinates tends to be reduced as the resolution is increased, since more experimental diffraction data is available for the model fitting and refinement. Thus, for example, more diffraction data can be collected from a crystal that diffracts to a resolution of 2.8 angstroms than from a crystal that diffracts to a lower resolution, such as 3.5 angstroms. Consequently, the refined structural coordinates will usually be more accurate when fitted and refined using data from a crystal that diffracts to higher resolution. The design of agonists, antagonists, and modulators for UPPS depends on the accuracy of the structural coordinates. If the coordinates are not sufficiently accurate, then the design process will be ineffective. In most cases, it is very difficult or impossible to collect sufficient diffraction data to define atomic coordinates precisely when the crystals diffract to a resolution of only 3.5 angstroms or poorer. Thus, in most cases, it is difficult to use X-ray structures in structure-based agonist and antagonist design when the X-ray structures are based on crystals that diffract to a resolution of only 3.5 angstroms or poorer. However, common experience has shown that crystals diffracting to 2.8 angstroms or better can yield X-ray structures with sufficient accuracy to greatly facilitate structure-based drug design. Further improvement in the resolution can further facilitate structure-based design, but the coordinates obtained at 2.8 angstroms resolution are generally adequate for most purposes.

Also, those of skill in the art will understand that UPPS proteins can adopt different

conformations when different agonists, antagonists, and modulators are bound. Subtle variations in the conformation can also occur when different agonists are bound, and when different antagonists are bound. These variations can be difficult or impossible to predict from a single X-ray structure. Generally, structure-based design of UPPS modulators depends to some degree on a knowledge of the differences in conformation that occur when agonists and antagonists are bound. Thus, structure-based modulator design is most facilitated by the availability of X-ray structures of complexes with potent agonists as well as potent antagonists.

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As used herein, the term "substantially pure" means that the polynucleotide or polypeptide is substantially free of the sequences and molecules with which it is associated in its natural state, and those molecules used in the isolation procedure. The term "substantially free" means that the sample is at least 50%, preferably at least 70%, more preferably 80% and most preferably 90% free of the materials and compounds with which is it associated in nature.

As used herein, the term "target cell" refers to a cell, into which it is desired to insert a nucleic acid sequence or polypeptide, or to otherwise effect a modification from conditions known to be standard in the unmodified cell. A nucleic acid sequence introduced into a target cell can be of variable length. Additionally, a nucleic acid sequence can enter a target cell as a component of a plasmid or other vector or as a naked sequence.

As used herein, the term "transcription" means a cellular process involving the interaction of an RNA polymerase with a gene that directs the expression as RNA of the structural information present in the coding sequences of the gene. The process includes, but is not limited to the following steps: (a) the transcription initiation, (b) transcript elongation, (c) transcript splicing, (d) transcript capping, (e) transcript termination, (f) transcript polyadenylation, (g) nuclear export of the transcript, (h) transcript editing, and (i) stabilizing the transcript.

As used herein, the term "transcription factor" means a cytoplasmic or nuclear protein which binds to such gene, or binds to an RNA transcript of such gene, or binds to another protein which binds to such gene or such RNA transcript or another protein which in turn binds to such gene or such RNA transcript, so as to thereby modulate expression of the gene. Such modulation can additionally be achieved by other mechanisms; the essence of "transcription factor for a gene" is that the level of transcription of the gene is altered in some way.

As used herein, the term "unit cell" means a basic parallelipiped shaped block. The entire volume of a crystal can be constructed by regular assembly of such blocks. Each unit

cell comprises a complete representation of the unit of pattern, the repetition of which builds up the crystal. Thus, the term "unit cell" means the fundamental portion of a crystal structure that is repeated infinitely by translation in three dimensions. A unit cell is characterized by three vectors a, b, and c, not located in one plane, which form the edges of a parallelepiped. Angles •, •, and • define the angles between the vectors: angle • is the angle between vectors b and c; angle • is the angle between vectors a and c; and angle • is the angle between vectors a and b. The entire volume of a crystal can be constructed by regular assembly of unit cells; each unit cell comprises a complete representation of the unit of pattern, the repetition of which builds up the crystal.

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As used herein, the term "mutant" or "mutation" carries its traditional connotation and means a change, inherited, naturally occurring or introduced, in a nucleic acid or polypeptide sequence, and is used in its sense as generally known to those of skill in the art. For example, a UPPS polypeptide, i.e., a polypeptide displaying the biological activity of wild-type UPPS activity, characterized by the replacement of at least one active-site amino acid from the wild-type prenyltransferase sequence. Such a mutant may be prepared, for example, by expression of the UPPS prenyltransferase cDNA previously altered in its coding sequence by oligonucleotide-directed mutagenesis.

UPPS mutants may also be generated by site-specific incorporation of unnatural amino acids into the UPPS protein using the general biosynthetic method of C. J. Noren et al, *Science*, 244:182-188 (1989). In this method, the codon encoding the amino acid of interest in wild-type UPPS is replaced by a "blank" nonsense codon, TAG, using oligonucleotide-directed mutagenesis. A suppressor directed against this codon is then chemically aminoacylated *in vitro* with the desired unnatural amino acid. The aminoacylated residue is then added to an *in vitro* translation system to yield a mutant UPPS enzyme with the site-specific incorporated unnatural amino acid.

Selenocysteine or selenomethionine may be incorporated into wild-type or mutant metallo UPPS prenyltransferase by expression of UPPS-encoding cDNAs in auxotrophic *E. coli* strains (W. A. Hendrickson et al, *EMBO J.*, 9(5):1665-1672 (1990)) or a normal strain grown in a medium supplemented with appropriate nutrients that will prevent endogenous synthesis of methionine. In either of these methods, the wild-type or mutated undecaprenyl pyrophosphate synthase cDNA may be expressed in a host organism on a growth medium depleted of either natural cysteine or methionine (or both) but enriched in selenocysteine or selenomethionine (or both).

The term "heavy atom derivative" refers to derivatives of UPPS produced by chemically modifying a crystal of UPPS. In practice, a native crystal is tretaed by

immersing it in a solution containing the desired metal salt, or organometallic compound, e.g., lead chloride, gold thiomalate, thimerosal or uranyl acetate, which upon diffusion into the protein crystal can bind to the protein. The location of the bound heavy metal atom site(s) can be determined by X-ray diffraction analysis of the treated crystal. This information, in turn, is used to generate the phase angle information needed to construct a three-dimensional electron density map from which a model of the atomic structure of the enzyme is derived (T. L. Blundel and N. L. Johnson, *Protein Crystallography*, Academic Press (1976)).

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The term "space group" refers to the arrangement of symmetry elements (i.e. molecules) throughout the crystal. There are only 132 possible arrangements, each one unique and identified by a symbol. The space group symbol is formed by a letter (P, F, I, C) and numbers with or without subscripts, for example: P2₁ 1222, C2₁2₁2₁ etc.

Methods of Identifying Inhibitors of UPPS from Streptococcus pneumoniae Crystalline Structure

An aspect of this invention involves a method for identifying inhibitors of a UPPS characterized by the crystal structure and novel active site described herein, and the crystal structures of the complexes with its substrates. The novel prenyltransferase crystalline structure of the invention permits the identification of inhibitors of prenyltransferase activity. Such inhibitors may be competitive, binding to all or a portion of the active site of UPPS; or non-competitive and bind to and inhibit undecaprenyl pyrophosphate synthase whether or not it is bound to another chemical entity.

One design approach is to probe a UPPS crystal of the invention with molecules composed of a variety of different chemical entities to determine optimal sites for interaction between candidate UPPS inhibitors and the enzyme. For example, high resolution X-ray diffraction data collected from crystals saturated with solvent allows the determination of where each type of solvent molecule binds. Small molecules that bind tightly to those sites can then be designed and synthesized and tested for a UPPS inhibitor activity (J. Travis, Science, 262:1374 (1993)).

This invention also enables the development of compounds that can isomerize to short-lived reaction intermediates in the chemical reaction of a substrate or other compound that binds to or with a UPPS. Thus, the time-dependent analysis of structural changes in a UPPS during its interaction with other molecules is permitted. The reaction intermediates of the UPPS can also be deduced from the reaction product in co-complex with a UPPS. Such information is useful to design improved analogues of known UPPS inhibitors or to design

novel classes of inhibitors based on the reaction intermediates of a UPPS enzyme and UPPS inhibitor co-complex. This provides a novel route for designing UPPS inhibitors with both high specificity and stability.

Another approach made possible by this invention, is to screen computationally small molecule data bases for chemical entities or compounds that can bind in whole, or in part, to a UPPS enzyme. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity or by estimated interaction energy (E. C. Meng et al, *J. Comp. Chem.*, 13:505-524 (1992)).

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Because UPPS may crystallize in more than one crystal form, the structure coordinates of UPPS, or portions thereof, as provided by this invention are particularly useful to solve the structure of those other crystal forms of UPPS. They may also be used to solve the structure of UPPS mutant co-complexes, or of the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of UPPS.

One method that may be employed for this purpose is molecular replacement. In this method, the unknown crystal structure, whether it is another crystal form of UPPS, a UPPS mutant, a UPPS co-complex, a UPPS from a different bacterial species, or the crystal of some other protein with significant amino acid sequence homology to any domain of UPPS, may be determined using the UPPS structure coordinates of this invention as provided in Figures 1-5 and Tables I - III. This method will provide an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information *ab initio*.

Thus, preferred UPPS structures provided herein permits the screening of known molecules and/or the designing of new molecules which bind to the structure, particularly at the binding pocket or active site, via the use of computerized evaluation systems. For example, computer modeling systems are available in which the sequence of a UPPS, and a UPPS structure (i.e., the atomic coordinates, bond distances between atoms in the active site region, etc. as provided by Tables I - III herein) may be input. Thus, a machine readable medium may be encoded with data representing the coordinates of Tables I - III. The computer then generates structural details of the site into which a test compound should bind, thereby enabling the determination of the complementary structural details of said test compound.

More particularly, the design of compounds that bind to or inhibit UPPS according to this invention generally involves consideration of two factors. First, the compound must be capable of physically and structurally associating with UPPS. Non-covalent molecular

interactions important in the association of UPPS with its substrate include hydrogen bonding, van der Waals, and hydrophobic interactions.

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Second, the compound must be able to assume a conformation that allows it to associate with UPPS. Although certain portions of the compound will not directly participate in this association with UPPS, those portions may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity or compound in relation to all or a portion of the binding site, e.g., binding pocket, active site, or substrate binding sites of UPPS, or the spacing between functional groups of a compound comprising several chemical entities that directly interact with UPPS.

Another approach made possible by this invention is to screen computationally small molecule databases for chemical entities or compounds that can bind in whole, or in part, to a UPPS enzyme. Details on this process and the results it can provide are now documented in the art. For a description of this type of technology please refer to PCT application WO 97/16177 published 09 May 1997; the techniques described there for computer modeling are incorporated herein by reference.

Once identified by the modeling techniques, the prenyltransferase inhibitor may be tested for bio-activity using standard techniques. For example, the structure of the invention may be used in enzymatic activity assays to determine the inhibitory activity of the compounds or binding assays using conventional formats to screen inhibitors. One particularly suitable assay format includes the enzyme-linked immunosorbent assay (herein "ELISA"). Other assay formats may be used; these assay formats are not a limitation on the present invention.

The potential inhibitory or binding effect of a chemical compound on UPPS may be analyzed prior to its actual synthesis and testing by the use of computer modelling techniques. If the theoretical structure of the given compound suggests insufficient interaction and association between it and UPPS, synthesis and testing of the compound is obviated. However, if computer modelling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to UPPS and inhibit using a suitable assay. In this manner, synthesis of inoperative compounds may be avoided.

An inhibitory or other binding compound of UPPS may be computationally evaluated and designed by means of a series of steps in that chemical entities or fragments are screened and selected for their ability to associate with the individual binding pockets or other areas of UPPS.

One skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with UPPS and more particularly with the individual binding pockets of the UPPS active site or accessory binding site. This process may begin by visual inspection of, for example, the active site on the computer screen based on the UPPS coordinates in Tables I-III. Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within an binding pocket or active site of UPPS. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics

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Specialized computer programs may also assist in the process of selecting fragments or chemical entities. These include:

forcefields, such as CHARMM and AMBER.

- 1. GRID (P. J. Goodford, "A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules", *J. Med. Chem.*, 28:849-857 (1985)). GRID is available from Oxford University, Oxford, UK.
- MCSS (A. Miranker and M. Karplus, "Functionality Maps of Binding Sites:
 A Multiple Copy Simultaneous Search Method", Proteins: Structure, Function and Genetics, 11:29-34 (1991)). MCSS is available from Molecular Simulations, Burlington, MA.
- 3. AUTODOCK (D. S. Goodsell and A. J. Olsen, "Automated Docking of Substrates to Proteins by Simulated Annealing", *Proteins: Structure, Function, and Genetics*, 8:195-202 (1990)). AUTODOCK is available from Scripps Research Institute, La Jolla, CA.
- DOCK (I. D. Kuntz et al., "A Geometric Approach to Macromolecule-Ligand Interactions", J. Mol. Biol., 161:269-288 (1982)). DOCK is available from University of California, San Francisco, CA.

In addition, other commercially available computer databases for small molecular compounds includes Cambridge Structural Database, Fine Chemical Database, and CONCORD, for a review see Rusinko, A., Chem. Des. Auto. News 8, 44-47 (1993).

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or inhibitor. Assembly may be proceed by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of UPPS. This would be followed by manual model building using software such as Quanta or Sybyl.

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include:

1. CAVEAT (P. A. Bartlett et al, "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules", in Molecular Recognition in Chemical and Biological Problems", Speical Pub., Royal Chem. Soc. 78, pp. 182-196 (1989)]. CAVEAT is available from the University of California, Berkeley, CA.

- 5 2. 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, CA). This area is reviewed in Y. C. Martin, "3D Database Searching in Drug Design," J. Med. Chem., 35:2145-2154 (1992).
 - 3. HOOK (available from Molecular Simulations, Burlington, MA).

 Instead of proceeding to build a UPPS inhibitor in a step-wise fashion one fragment or chemical entity at a time as described above, inhibitory or other UPPS binding compounds may be designed as a whole or "de novo" using either an empty active site or

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- 1. LUDI (H.J. Bohm, "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", *J. Comp. Aid. Molec. Design*, <u>6</u>:61-78 (1992)). LUDI is available from Biosym Technologies, San Diego, CA.
- 2. LEGEND (Y. Nishibata and A. Itai, *Tetrahedron*, 47:8985 (1991)). LEGEND is available from Molecular Simulations, Burlington, MA.

optionally including some portion(s) of a known ligand(s). These methods include:

3. LeapFrog (available from Tripos Associates, St. Louis, MO).

Other molecular modelling techniques may also be employed in accordance with
this invention. See, e.g., N. C. Cohen et al, "Molecular Modeling Software and Methods for
Medicinal Chemistry", J. Med. Chem., 33:883-894 (1990). See also, M. A. Navia and M. A.
Murcko, "The Use of Structural Information in Drug Design", Current Opinions in
Structural Biology, 2:202-210 (1992). For example, where the structures of test compounds
are known, a model of the test compound may be superimposed over the model of the
structure of the invention. Numerous methods and techniques are known in the art for
performing this step, any of which may be used. See, e.g., P.S. Farmer, Drug Design,
Ariens, E.J., ed., Vol. 10, pp 119-143 (Academic Press, New York, 1980); U.S. Patent No.
5,331,573; U.S. Patent No. 5,500,807; C. Verlinde, Structure, 2:577-587 (1994); and I. D.
Kuntz, Science, 257:1078-1082 (1992). The model building techniques and computer
evaluation systems described herein are not a limitation on the present invention.

Thus, using these computer evaluation systems, a large number of compounds may be quickly and easily examined and expensive and lengthy biochemical testing avoided.

Moreover, the need for actual synthesis of many compounds is effectively eliminated.

In another aspect, the undecaprenyl pyrophosphate synthase structure of the invention permit the design and identification of synthetic compounds and/or other

molecules which are characterized by the conformation of the undecaprenyl pyrophosphate synthase of the invention. Using known computer systems, the coordinates of the undecaprenyl pyrophosphate synthase structure of the invention may be provided in machine readable form, the test compounds designed and/or screened and their conformations superimposed on the structure of the undecaprenyl pyrophosphate synthase of the invention. Subsequently, suitable candidates identified as above may be screened for the desired undecaprenyl pyrophosphate synthase inhibitory bio-activity, stability, and the like.

Once identified and screened for biological activity, these inhibitors may be used therapeutically or prophylactically to block undecaprenyl pyrophosphate synthase activity, and thus, overcome bacterial resistance to antibiotics, for example, of the beta-lactam class, eg. imipenem, penicillins, cephalosporins, etc. by using an entirely different mechanism of attacking bacteria in diseases produced by bacterial infection.

15 Abbreviations used herin

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	TIDOTO TRACTORIS GOOD	
	ATP	adenosine triphosphate
	ADP	adenosine diphosphate
	AR	androgen receptor
	CAT	chloramphenicol acyltransferase
20	CBP	CREB binding protein
٠.	cDNA	complementary DNA
	DBD	DNA binding domain
	DMSO	dimethyl sulfoxide
	DNA	deoxyribonucleic acid
25	DTT	dithiothreitol
	EDTA	ethylenediaminetetraacetic acid
	ER	estrogen receptor
	FPP	farnesyl pyrophosphate
	GST	glutathione S-transferase
30	HEPES	N-2-Hydroxyethylpiperazine-N'-2-ethanesulfonic acid
	HSP	heat shock protein
	IPP	Isopentenyl pyrophosphate
	kDa	kilodalton(s)
	LBD	ligand binding domain
35	MR	mineralcorticoid receptor

	NDP	nucleotide diphosphate
	NID	nuclear receptor interaction domain
	NTP	nucleotide triphosphate
	PAGE	polyacrylamide gel electrophoresis
5	PCR	polymerase chain reaction
	pI	isoelectric point
	PPAR	peroxisome proliferator-activated receptor
	PR	progesterone receptor
	RAR	retinoid acid receptor
10	RXR	retinoid X receptor
	SDS	sodium dodecyl sulfate
	SDS-PAGE	sodium dodecyl sulfate polyacrylamide gel electrophoresis
	TIF2	transcription intermediary factor 2
	TR	thyroid receptor
15	UPPS	undecaprenyl pyrophosphate synthase
4	VDR	vitamin D receptor

Amino Acid Abbreviations used herein

	Single-Letter Code	Three-Letter Code	<u>Name</u>
20	Α	Ala	Alanine
	V	Val	Valine
	L	Leu	Leucine
	I	Ile	Isoleucine
	. P	Pro	Proline
25	F	Phe	Phenylalanine
	· W	Тгр	Tryptophan
	M	Met	Methionine
	G	Gly	Glycine
	S	Ser	Serine
30	T	Thr	Threonine
	С	Cys	Cysteine
	Y	Tyr	Tyrosine
	N	Asn	Asparagine
	Q	Gln	Glutamine
35	D	Asp	Aspartic Acid

WO 03/048733		PCT/US02/38715	
Е	Glu	Glutamic Acid	

K	100	Lys	Lysine
R		Arg	Arginine
H		His	Histidine

Functionally Equivalent Codons

	Amino Acid			Codons
•	Alanine	Ala	Α	GCA GCC GCG GCU
	Cysteine	Cys	C	UGC UGU
5	Aspartic Acid	Asp	D	GAC GAU
	Glumatic acid	Glu	E	GAA GAG
	Phenylalanine	Phe	F	ບບດຸດກາ
	Glycine	Gly	G	GGA GGC GGG GGU
	Histidine	His	\mathbf{H}	CAC CAU
10	Isoleucine	Ile	I	AUA AUC AUU
	Lysine	Lys	K	AAA AAG
	Methionine	Met	M	AUG
	Asparagine	Asn	· N	AAC AAU
	Proline	Pro	P	CCA CCC CCG CCU
	Glutamine	Gln	Q	CAA CAG
15	Threonine	Thr	T	ACA ACC ACG ACU
•	Valine	Val	V	GUA GUC GUG GUU
	Tryptophan	Trp	W	UGG
	Tyrosine	Tyr	Y	UAC UAU
	Leucine	Leu	$^{\prime}\mathbf{L}$	UUA UUG CUA CUC CUG CUU
20	Arginine	Arg	R	AGA AGG CGA CGC CGG CGU
	Serine	Ser	S	ACG AGU UCA UCC UCG UCU

The following examples illustrate various aspects of this invention. These examples do not limit the scope of this invention that is defined by the appended claims.

Example 1- Expression and purification of UPPS prenyltransferase from Streptococcus pneumoniae in Escherichia coli

UPPS from Streptococcus pneumoniae with an additional 20 residues at the amino terminus that include the hexa-histidine tag was over expressed in E. coli, strain BL21(DE3), and purified by NiNTA (nickel nitrilo-tri-acetic acid) column. A plasmid pET28-UPPS was transformed into E. coli BL21 (DE3). For expression E. coli BL21 (pET28-UPPS) was grown at 37 °C in LB medium containing 1% glucose and 50 ug/ml kanamycin to OD600 0.5 and then induced with 1 mM IPTG for 3 hrs. The induced cultures

were harvested by centrifugation. The cell paste was suspended in 25 ml Buffer A (10mM imidazole, 50mM Na-phosphate, 0.5M NaCl pH7.5) containing 0.1mg/ml of lysozyme. After incubating on ice 30 min, the cell suspension was put through 4 cycles of sonication, freeze and thaw. The lysate was centrifuged and the supernatant applied to the NiNTA column. The column was washed with 18 ml of Buffer A and 12.5ml of Buffer B (100 mM imidazole, 50mM Na-phosphate, 0.5M NaCl pH7.5). The His-tagged UPPS was eluted with 10 ml of Buffer C (500 mM imidazole, 50mM Na-phosphate, 0.5M NaCl pH7.5). The eluted His-UPPS was dialyzed overnight at 4 °C against 2L of 50mM Tris-HCl pH 7.5, 0.2M NaCl and 1mM EDTA. The soluble polypeptide includes 272 amino acid residues with a molecular weight of 29,000. This product was greater than 95% pure by SDS PAGE, has the desired enzymatic activity, and N-terminal amino acid analysis confirmed its identity.

1.A. Measurement of UPPS activity

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Enzymatic activity of UPPS was assayed by measuring the incorporation of (1-14C)IPP (isopentenyl diphosphate) into butanol-soluble materials from the condensations of FPP and (1-14C)IPP using a butanol extraction assay (Shimizu et al. 1998). A typical assay of 100 ul contained 100 mM Tris-HCl, pH7.5, 50 mM KCl, 0.5 mM MgCl2, 0.05% Triton X-100, 0.5 uM FPP, 3.6 uM (1-14C)IPP, and 6 nM purified *S. pneumoniae* His-UPPS. The reaction was incubated at 25 °C for 25 min and stopped by addition of EDTA to 50 mM. The reaction was extracted with equal volume of 1-butanol and the radioactivity in the butanol phase was measured with a liquid scintillation counter (Shimizu, N., T. Koyama, and K. Ogura. (1998) *J Biol. Chem.* 273:19476-19481).

25 1.B. Ligand binding to UPPS

It is also possible to define ligand interactions with UPPS in experiments that are not dependent upon enzyme catalyzed turnover of substrates. This type of experiment can be done in a number of ways:

30 1.B.1. Effects of ligand binding upon enzyme intrinsic fluorescence (e.g. of tryptophan)
Binding of either natural ligands or inhibitors may result in enzyme conformational changes which alter enzyme fluorescence. Using stopped-flow fluorescence equipment, this can be used to define the microscopic rate constants that describe binding. Alternatively, steady-state fluorescence titration methods can yield the overall dissociation constant for binding in the same way that these are accessed through enzyme inhibition experiments.

Example 2 <u>Crystallization</u>, <u>structure determination</u> and <u>refinement of a crystal structure of UPPS from Streptococcus pneumoniae</u>

2.A. Crystallization '

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Single crystals of native UPPS grew from sitting or hanging drops prepared by mixing 2 uL protein (9.5 mg/ml in 50mM Tris-HCl, pH 7.5, 0.2M NaCl, 1mM EDTA) with 2µL of reservoir solution containing either 10-20% ethanol, 0.1M Tris-HCl, pH 8.5 or 4-5% PEG6000, 0.1M HEPES, pH 7.5. The drops were left to equilibrate at room temperature against 500µL of the reservoir solution. The crystals belong to the orthorhombic crystalline form having a space group $P2_12_12_1$ with unit cell parameters: $a = 59.6 \text{\AA}$, $b = 118.0 \text{\AA}$, $c = 118.0 \text{\AA}$ 178.2Å, and two 60 kDa dimers in the asymmetric unit. Some crystals were found to belong to the orthorhombic crystalline form having a space group I2₁2₁2₁ with the similar cell parameters as the primitive cell. In the primitive cell, a pseudo-translation of nearly 1/2, 1/2, 1/2 along the cell edges, results in a diffraction pattern in which the h + k + l = odd are, on the average, markedly weaker than the h + k + l = even reflections resulting in a pseudo body centered lattice. The crystals were quickly transferred to a solution of mother liquor containing 30% xylitol as cryo-protective agent and flash frozen under the cold stream before data collection. The Se-Met substituted protein was expressed in E. coli fed with an amino acid mixture that inhibited the endogenous biosynthesis of methionine and forced the uptake of selenium-labeled methionine from the medium. The protein was crystallized under similar conditions with the exception that the crystallization drops were flushed with argon gas before sealing them in order to prevent oxidation. The crystal structure of UPPS in complex with IPP was determined using native crystals soaked at room temperature for 20-30 minutes in mother liquor containing 2-3mM IPP and 2mM MgCl₂. The co-crystals of UPPS in complex with the substrate IPP crystals belong to the orthorhombic crystalline form having the space groups P2₁2₁2₁ and I2₁2₁2₁, similar to the native crystal. The cocrystals of UPPS in complex with the substrate FPP were grown at room temperature from sitting drops prepared by mixing 2uL of protein solution (~10mg/ml, 2mM FPP, 1,mM MgCl2, 50mM Tris-HCl pH 7.5 and 200mM NaCl) with 2uL of reservoir solution containing 100mM sodium cacodylate, pH 6.4, 120-240 mM sodium acetate. These crystals belong to the monoclinic crystalline form having a space group P21 with unit cell dimensions a = 58.1 Å, b = 44.6 Å, c = 115.5 Å, $\beta = 98.7^{\circ}$.

2.B. X-ray diffraction data collection

A native UPPS crystal structure was determined by multiwavelength anomalous diffraction, MAD, using the K absorption edge of selenium incorporated into the amino acid methionine. Three diffraction data sets to 2.3Å resolution were collected at the NSLS's X12C beamline. The wavelengths were determined by analyzing the x-ray fluorescence of the UPPS crystal around the selenium absorption edge. These correspond to the peak (0.9795Å), the inflection point (0.9791Å) and at a remote wavelength on the high-energy side of the edge (0.9500Å). Diffraction intensities from each wavelength were independently integrated, merged and scaled using DENZO/SCALEPACK (Otwinowsky, et al. (1999) Methods in Enzymology Vol. 267). Diffraction data from UPPS in complex with FPP or IPP were collected at the 17ID beamline at the Advanced Photon Source, APS, at Argonne National Laboratory, using 1.000Å wavelength.

2.C. Structure Determination

A selenium substructure was determined by automatic Patterson map peak search and peak correlation implemented in the program SOLVE (Terwilliger, T. C., and Berendsen, J. (1999) Acta Crystallogr. D55: 849-861). A Fourier map was calculated to 2.7Å resolution using phases calculated from 15 of the possible 24 Se sites in the asymmetric unit. After solvent modification, this map afforder the determination of the boundaries of the four monomers and tracing of the polypeptide chains. The tracing was used to find the rotation and translation transformations used in 4-fold electron density averaging (CCP4, DM). The improved, averaged map was also used in tracing of the chains.

2.D. Model Building and Refinement

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This averaged electron density map was of high quality and afforded the complete tracing of the four molecules using the interactive computer graphics program O (Jones, T.A. et al. (1991) Acta Crystallogr. A47: 110-119). The initial model was refined against diffraction data collected at the remote wavelength by successive rounds of simulated annealing with torsion angle dynamics, positional refinement and restrained B-factor refinement using CNS (A. Brunger et al., Science, 235: 458-460 (1987)) followed by manual intervention. The refinement and manual rebuilding was monitored by the quality of the 2Fo-Fc and Fo-Fc electron density maps and the value of the crystallographic R and R_{free}. At the beginning of the refinement, the four molecules in the asymmetric unit (A, B C, and D) were forced to obey strict non-crystallographic symmetry. This constraint was released as the refinement proceeded.

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A final R is 0.20 and the R_{free} is 0.25 for 53,642 reflections to 2.3Å resolution. The rms deviation from the reference bond lengths and bond angles (Engh & Huber (1991) Acta Crystallogr. A47: 392-400) are 0.01 and 1.4, respectively. The refined model includes residues 17-72, 77-248 in molecule A, 17-72, 79-246 in molecule B, 17-73, 77-248 in molecule C and 18-73, 78-246 in molecule D according to the amino acid sequence SEQ ID NO:1. The N-terminal residues 1-16 were disordered in the four molecules. Also were disordered the residues in the vicinity of the loop formed by amino acids 72-80. A number of conserved amino acids that may form part of the active site (see below) are located in this region. The six residues 247-252 at the C-terminus were also disordered. In the refined model, all the main chain conformations fall in the "allowed" regions of the Ramachandran plot. Molecules A and B form one of the dimers and molecules C and D the second dimer in the asymmetric unit. The Ca-carbon atoms of the two pairs of molecules in each dimer, molecules A and B, and C and D, superimpose with a rms deviation of 1.2Å and 1.1Å, respectively, with very large differences at the N- (6.1Å) and C-termini (1.5Å), the turn formed by residues 35-41 (1.2Å), the long helix formed by residues 79-104 (7.1Å), the short turn formed by residues 115-127 (2.2Å), and residues 157-171 (1.7Å) that form an α -helix and a turn. Omitting these residues from the comparison gives a rms of 0.3Å or both pairs of molecules. The turn formed by residues 35-41 (1.2Å) in molecule A has no crystal contacts or contacts with the partner in the dimer, however, in molecule B it is making contacts with the sane region in molecule D. The long helix from 79-104 is not making contacts in molecules A or D but in C is contacting residues in the region of B177, and in B is contacting D117 of a symmetry related molecule; this region leads to a disordered loop that may be involved in substrate binding. B115 region is in contact with symmetry related D119-D121, and D115 is contacting symmetry related B85-B88 region. A166 is in contact with symmetry related B240, C166 is in contact with symmetry related D240, but neither B166 nor D166 are making any crystal contacts.

A crystal structure of a UPPS in complex with FPP was determined by molecular replacement with the program package AMoRe (Navaza, J. (1994) Acta Cryst. A50, 157-163) using the native structure as search model and refined as described before. The cross rotation and translation searches were carried using data from 20Å to 4Å resolution and a radius of integration of 20Å. The top two solutions of the cross rotation function corresponding to the tow molecules in the dimer in the asymmetric unit were unambiguously discriminated from the noise peaks. The search for the correct translation for each molecule in the asymmetric unit produced a solution for the tetramer with an R-factor

of 0.60 and a correlation coefficient of 0.34 after rigid body refinement in. The crystal structure of the complex with IPP was determined by Fourier methods.

All documents cited herein and patent applications to which priority is claimed are incorporated by reference herein in their entirety. This invention is not to be limited in scope by the specific embodiments described herein. Indeed, various modifications of the invention in addition to those described herein will become apparent to those skilled in the art from the foregoing description. Such modifications are intended to fall within the scope of the appended claims. The disclosures of the patents, patent applications and publications cited herein are incorporated by reference in their entireties.

SEQUENCE LISTING

```
(1) GENERAL INFORMATION:
            (i) APPLICANT: Néstor O. Concha, and Cheryl A. Janson
  5
            (ii) TITLE OF INVENTION: Novel UPPS Enzyme
            (iii) NUMBER OF SEQUENCES: 1
            (iv) CORRESPONDENCE ADDRESS:
                  (A) ADDRESSEE: GlaxoSmithKline Corporation
                        (B) STREET: 709 Swedeland Road - P.O. Box 1539
 10
                        (C) CITY: King of Prussia
                        (D) STATE: Pennsylvania
                        (E) COUNTRY: USA
                        (F) ZIP: 19406-2799
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           (v) COMPUTER READABLE FORM:
                  (A) MEDIUM TYPE: Floppy disk
                  (B) COMPUTER: IBM PC compatible
                  (C) OPERATING SYSTEM:
 20
                  (D) SOFTWARE:
          (vi) CURRENT APPLICATION DATA:
                  (A) APPLICATION NUMBER:
                  (B) FILING DATE:
 25
                  (C) CLASSIFICATION:
         (vii) PRIOR APPLICATION DATA:
                  (A) APPLICATION NUMBER:
                  (B) FILING DATE:
 30
                  (A) APPLICATION NUMBER:
                  (B) FILING DATE:
        (viii) ATTORNEY/AGENT INFORMATION:
 35
                  (A) NAME:
                  (B) REGISTRATION NUMBER:
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(C) REFERENCE/DOCKET NUMBER:

	(ix) TE	LECOMMUNICA	rion inform	ATION:	
		(A) TELEPHO	ONE:		0 0
		(B) TELEFA	X:		
5					
	(2) INFORMA	TION FOR SE	Q ID NO:1:		
	(i) S	EQUENCE CHA	RACTERISTIC	S:	
10	, ,	•	LENGTH: 272		s
		(B)	TYPE: amino	acid	•
		(C)	STRANDEDNES	SS:	
		(D)	TOPOLOGY: 1	inear	
		•	1		Carlos Anno 1997
15	(ii)	MOLECULE TY	PE: protein	1	4
				· · · · · · · · · · · · · · · · · · ·	
•	(iii)	SEQUENCE I	ESCRIPTION:	SEQ ID NO:	1:
20	-20	-10	1	11	21
20			MFGFFKKDKĄ	VEVEVPTQVP-	AHIGIIMDGN
	31	41	51	61	71
		RVFGHKAGME	ALQTVTKAAN	KLGVKVITVY	AFSTENWTRP
25			•		*
	81	91	101	111	121
	DQEVKFIMNL	PVEEADNAAL	ELHANNVKIQ	MIGETORLPK	OLL FULL VAF
	131	141	151	161	171
30			AEITQALKLI	SQDVLDAKIN	PGDITEELIG
·			201	211	221
	181	191	201	211	YFTDTLWPDF
	MAPLIOHPSK	DUKDEDDITIK	TOGETKIDIAL	TIMZGUIDID	
25	021	2.41	251		•

DEAALQEAIL AYNRRHRRFG GV

Figure 1A

Figure 1B

Figure 2A

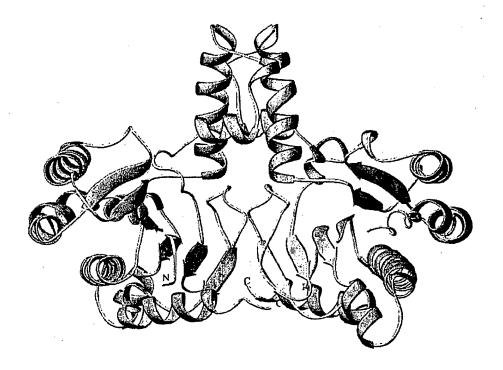


Figure 2B

UPS (S. pneumoniae)

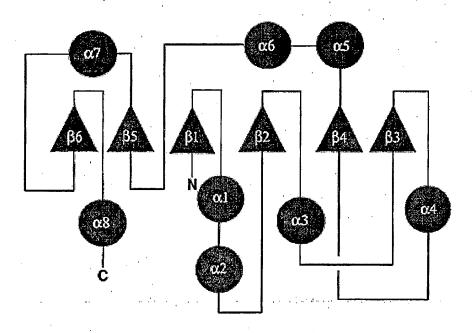


Figure 3A

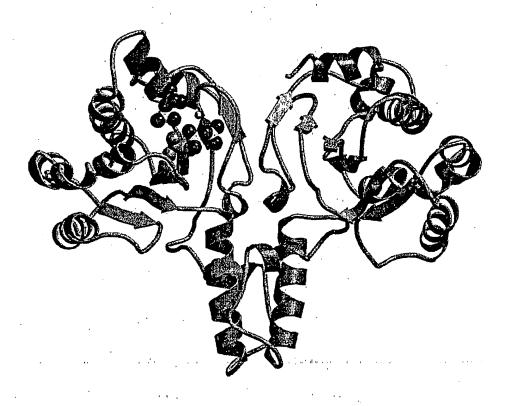


Figure 3B

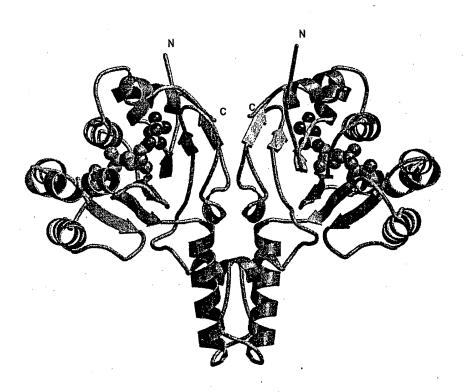


Figure 4A

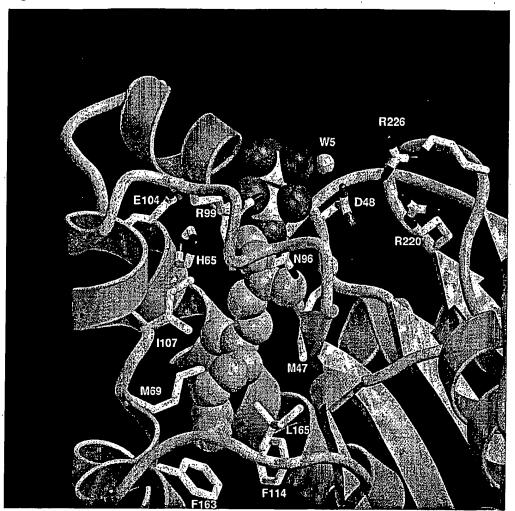


Figure 4B

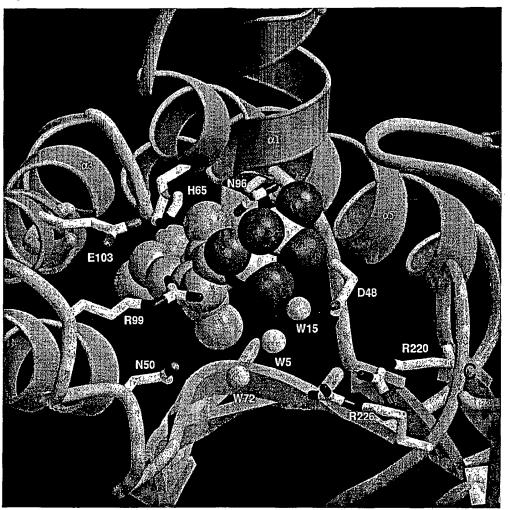


Figure 5

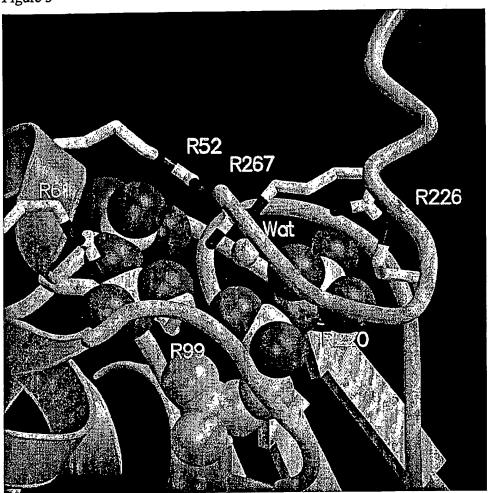


TABLE I

Table IA. Atomic coordinates of native UPPS structure

5 Table IB. Atomic coordinates of active of UPPS in complex with FPP Table IC. Atomic coordinates of active of UPPS in complex with IPP

TABLE II

Table IIA. Interatomic distances in an active site of the native UPPS

Table IIB. Interatomic distances in an active site of UPPS in complex with FPP Table IIC. Interatomic distances in an active site of UPPS in complex with IPP

TABLE III

Table IIIA. Interatomic angles in an active site of the native UPPS

Table IIIB. Interatomic angles in an active of UPPS in complex with FPP Table IIIC. Interatomic angles in an active of UPPS in complex with IPP

Legend:

- Under the heading ATOM appears a "atom number" (e.g. 1,2,3,4...etc) and the "atom name" (e.g. CA, CB, N,... etc) such that to each "atom name" in the coordinate list corresponds an "atom number".
- Under the heading RESIDUE appears a three-letter "residue name" (e.g. THR, ASP, etc), a "chain identifier" represented by a capital letter (e.g. A, B, C D, etc) and a "residue number", such that to each residue (or amino acid) in the amino acid sequence of the particular protein in the structure corresponds a name that identifies it, a number according to its position along the amino acid sequence, and a chain name. The chain name identifies a particular molecule in the crystal structure. For instance, if there are more than one molecule that form the unit that is repeated throughout the crystal lattice, then each unit is identified
 as molecule A, or molecule B, or molecule C, etc.
 - 3. Under the headings X, Y, or Z appear the Cartesian coordinates of the atoms in the structure.

4. Under the heading OCC appears the "occupancy factor" for each atom. If the entity is present and observed in the structure then occupancy of 1.00 is assigned to it. If the atom is present but not observed, occupancy of 0.00 is assigned to it. Also, factors between 0.00 and 1.00 are also acceptable and represent the degree of confidence in observing that atom a that particular position.

5. Under the heading B appears the "B-factor" or "temperature factor" which can adopt, in principle, any value. It is meant to represent the atomic displacement around that position.

10 Table IAAtomic coordinates of native UPPS

5

										00	00	
	CRY	rst1	59.6	00	118.0	000	178.	200 9	0.00	90.0	•	0.00
	<u>ATC</u>	MC	RESID	<u>UE</u>		<u>X</u>		X	<u>Z</u>		. <u>0cc</u>	<u>B</u>
	1	CB ·	THR A	17		18.4		87.195				93.58
15	2	OG1	THR A	17		18.5		87.203		,	•	94.14
	3	CG2	THR A	17		17.1	90	88.014	103	.149		93.23
	4	С	THR A	17		19.6	37	84.999	103	.347	1.00	89.94
	5	0	THR A	17		20.5	25	85.538	104	.017	1.00	91.11
	6	N	THR A	17	•	17.1	69	85.002	103	.724	1.00	90.66
20.	7	CA	THR A	17	,	18.3		85.723			1.00	91.60
	8	N	GLN A	18		19.7	61	83.783	102	.808	1.00	86.41
	9.	CA	GLN A	18	- 1	20.9	49	82.945	102	.991		80.31
	10	СВ	GLN A	. 18	В	22.	219	83.75	7 10	2:767	1.00	83.93
	11	CG	GLN A	. 1	8	22.	233	84.54	8 10	1.482	1.00	89.19
25	12	CD	GLN A	. 1	8	23.	150	85.74	17 10	1.583	1.00	94.65
	13	OE:	L GLN A	1	8	24.	334	85.61	2 10	1.914	1.00	95.46
	14	NE	2 GLN A	1	8	22.	608	86.93	34. 10	1.306	1.00	95.13
	15	С	GLN A	1	8	20.	918	82.43	33 10	4.429	1.00	73.54
	16	0	GLN A	1	8	21.	875	81.84	16 10	4.922	1.00	71.59
30	17	N	VAL A	1	9	19.	793	82.67	78 10	5.085	1.00	0 64.52
	18	CA	VAL F	1	9	19.	567	82.27	72 10	6.464	1.00	56.20
	19	СВ	VAL A	1	9	18.	912	83.44	15 10	7.244	1.0	53.44
	20	CG	1 VAL A	1	9	18.	089	82.93	35 10	8.392	1.0	0 51.55
	21	CG	2 VAL A	1	9	19.	991	84.38	33 10	7.750	1.0	0 55.06
35	22	С	VAL A	1	9	18.	667	81.02	24 10	6.548	1.0	0 50.21
	23	0	VAL A	1	9	17.	570	80.99	97 10	5.979	1.0	0 47.54
	24	N	PRO P	A 2	0	19.	132	79.9	67 10	7.243	1.0	0 42.84
	25	CD	PRO A	A 2	0	20.	450	79.7	72 10	7.880	1.0	0 36.61
	26	CA	PRO A	A 2	0	18.	304	78.7	63 10	7.358	1.0	0 35.73
40	27	СВ	PRO A	A 2	0	19.	193	77.8	08 10	8.161	1.0	0 36.35

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78.727 108.916
                                                        1.00 33.42
             PRO A
                     20
                              20.132
     28
        CG
                                                        1.00 35.84
                                      79.119 108.063
         Ċ
             PRO A
                     20
                              16.998
     29
                                                        1.00 41.13
                                      79.851 109.040
                     20
                              17.004
     30
             PRO A
         0
                                                        1.00 34.58
                                      78.607 107.572
                              15.877
             ALA A
                    . 21
     31
         Ν
                                                        1.00 30.24
                                      78.932 108.153
5
                              14.580
     32
         CA
            ALA A
                     21
                                                        1.00 28.08
                              13.469
                                       78.609 107.158
         CB
             ALA A
                     21
     33
                                                        1.00 35.80
                              14.256
                                       78.267 109.474
     34
         С
             ALA A
                     21
                                                        1.00 32.51
                                       78.805 110.261
                     21
                              13.469
     35
         0
             ALA A
                                       77.076 109.694
                                                        1.00 30.51
                              14.811
                     22
     36
         N
              HIS A
                                                        1.00 24.73
10
                              14.577
                                       76.339 110.925
             HIS A
                     22
         CA
     37
                                                        1.00 24.49
             HIS A
                                       75.232 110.678
         СВ
                              13.542
     38
                     22
                                                        1.00 17.70
                                       74.430 111.893
              HIS A
                     22
                              13,197
     39
         CG
                                                        1.00 23.53
                              13.751
                                       74.389 113.130
         CD2 HIS A
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     40
                                                        1.00 15.36
                                       73.555 111.921
         ND1 HIS A
                     22
                              12.134
     41
                                                        1.00 22.80
                                       73.011 113.122
15
                              12.041
     42
         CE1 HIS A
                     22
                                                        1.00 19.49
                              13.010
                                       73.502 113.878
         NE2 HIS A
                     22
     43
                              15.911
                                       75.772 111.420
                                                        1.00 31.35
              HIS A
                     22
         С
     44
                                       74.987 110.731
                                                        1.00 29.44
                              16.583
     45
         0
              HIS A
                     22
                                                        1.00 32.00
                              16.309
                                       76.213 112.608
                     23
              ILE A
     46
         N
                                                        1.00 28.24
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                              17.561
                                       75.789 113.215
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              ILE A
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                                       76.991 113.554
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         CB
              ILE A
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                                                        1.00 23.27
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                                       76.532 114.171
         CG2 ILE A
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                              18.652
                                       77.826 112.294
     50
         CG1 ILE A
                     23
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                                       78.959 112.501
                                                        1.00 33.77
     51
         CD1 ILE A
                     23
                                                        1.00 29.56
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                                       75.034 114.512
25
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         С
              ILE A
                     23
                                       75.551 115.412
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     53
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              ILE A
                                       73.809 114.595
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              GLY A
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              GLY A
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                                       73.238 116.624
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              GLY A
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              ILE A
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          CG1 ILE A
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              ILE A
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              ILE A
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                                       71.146 121.402
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              ILE A
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          CG2 ILE A
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          CG1 ILE A
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                               21.103
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              ILE A
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              ILE A
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                                       72.551 123.378
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              MET A
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                              22.293
 5
     75
          CA
              MET A
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                                       74.337 125.036
                              21.344
              MET A
                      27
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          CB
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                                       75.121 124.084
                      27
                              20.458
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              MET A
          CG
                                                        1.00 43.39
                                       76.248 124.852
     78 · SD
              MET A
                      27
                              19.237
                                                        1.00 18.61
                                       75.134 125.772
                              18.191
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              MET A
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                              23.016
10
                      27
          С
              MET A
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              MET A
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                                       70.232 125.159
          СВ
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                                                         1.00 40.92
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              ASP A
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                                       69.270 127.278
          OD1 ASP A
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                                       68.050 125.474
          OD2 ASP A
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              ASP A
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      88
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              GLY A
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              GLY A
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          CB
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                               24.568
          ND2 ASN A
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      99
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                                        74.167 132.229
30
      100
           С
                ASN A
                       30
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                                        74.980 132.873
                                27.595
                ASN A
      101
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                       30
                                                          1.00 42.35
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                       31
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                GLY A
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      102
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                                        72.369 133.710
                                27.575
                GLY A
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      103
           CA
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                                         72.587 133.617
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           С
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                       31
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                ARG A
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                                         72.294 132.234
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                                31.092
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                                         71.837 130.810
      108
           CB
                ARG A
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                                         70.865 130.693
           CG
                ARG A
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                                32.571
40
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                ARG A
                       32
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           NE
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                        32
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            CZ
                ARG A
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            NH1 ARG A
      113
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114
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               ARG A
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     118
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     119
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               TRP A
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          CG
               TRP A
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                               29.468
          CE2 TRP A
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                      33
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10
     123
          CE3 TRP A
                      33
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                                       79.214 133.143
                                                        1.00 52.10
     124
          CD1 TRP A
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                                       78.884 130.010
                                                        1.00 46.04
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          NE1 TRP A
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                                       80.238 130.185
                                                        1.00 49.62
     126
          CZ2 TRP A
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                               29.453
                                       81.705 131.954
                                                        1.00 51.56
     127
          CZ3 TRP A
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                               28.431
                                       80.425 133.743
                                                        1.00 52.07
15
     128
          CH2 TRP A
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                                                        1.00 52.75
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          С
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20
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              ARG A
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	167	CC	NDC	ת	37	32.527	80.387	134.902	1.00	63.20
	157		ARG		37	33.261		134.440		66.92
	158 159	CD NE	ARG ARG		37	32.981		133.044		
	160		ARG		37	33.178		132.027		74.26
5		NH1			37	33.649		132.247		73.92
3	161				37	32.926		130.783		75.48
	162		ARG			34.096		138.220		60.36
	163	С	ARG		37			139.026		63.86
	164	0	ARG		37			138.599		62.29
. 10	165	N	MET		38	34.345		140.011		64.24
10	166	CA	MET		38	34.369		140.724		67.10
	167	CB	MET		38	35.506	•			70.38
	168	CG	MET		38	36.885		140.280		77.34
	169	SD	MET		38	37.169		140.705		76.14
1.5	170	CE	MET		38	38.285		142,112		63.85
15	171	С	MET		38	33.050		140.716		
4	172	0	MET		38	33.003		141.939		65.90
	173	N	GLN		39	31.985		139.944		63.31
	174	CA	GLN		39	30.671		140.492		62.45
	175	CB	GLN		39	30.023		139.648		61.29
20	176	CG	GLN		39	30.575		139.923		69.13
	177	CD	GLN	A	39	30.115		141.266		76.78
	178	OE1	GLN	A	39	28.943		141.444		81.67
	179	NE2	GLN	A	39	31.026	1	142.228		80.44
	180	С	GLN	A	39	29.767		140.536		62.86
25	181	0	GLN	A	39	30.064		139.915	•	63.48
	182	N	PRO	A	40	28.649	77.133	141.279		64.92
	183	CD	PRO	A	40	28.105		142.059		65.41
	184	CA	PRO	A	40	27.753		141.343		65.47
	185	CB	PRO	A	40	26.764		142.442		62.80
30	186	CG	PRO	A	40	26.657	77.854	142.265		64.53
	187	С	PRO	A	40	27.072		139.987		65.74
	188	0	PRO	A	40	26.856		139.219		64.28
	189	N	ARG	A	41	26.747		139.694		64.20
	190	CA	ARG	Α.	41	26.098		138.434	1.00	66.35
35	191	CB	ARG	A	41	25.553		138.478		69.33
	192	CG	ARG	A	41	26.592	71.590	138.246		78.61
	193	CD	ARG	A	41	25.997	70.436	137.431		86.11
	194	NE	ARG	A	41	25.524	70.896	136.120	1.00	92.86
	195	CZ	ARG	A	41	24.937	70.125	135.204	1.00	95.17
40	196	NH1	ARG	A	41	24.737	68.836	135.439	1.00	98.23
	197	NH2	ARG	A	41	24.542	70.646	134.048	1.00	93.83
	198	С	ARG	A	41	24.956	75.058	138.088	1.00	65.18
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	244	С	AL.	ΑА	47		23.592	81.16	9 130.691	1.00	41.82
	245	0	AL	A A	47		23.613	81.80	1 129.625	1.00	42.67
	246	N	GL.	Y' A	4.8		23.059	79.95	5,130.809	1.00	37.99
5	247	CA	GL.	Y. A	48		22.467	79.28	5 129.671	1.00	39.35
	248	С	GL	Y A	48		21.180	79.92	L 129.164	1.00	42.61
	249	0	GL:	Y A	48	,	20.954	79.943	3 127.950	1.00	42.20
	250	N	ME	ΓА	49		20.330	80.421	130.068	1.00	42.02
	251	CA	ME	ΓA	49	,	19.071	81.054	129.659	1.00	43.54
10	252	СВ	ME	r A	49		18.151	81.303	3 130.865	1.00	43.46
	253	CG	ME	ΓA	4'9		17.787	80.066	131.668	0.50	43.91
	254	SD	ME	ΓА	49		16.447	80.362	132.865	0.50	50.86
	255	CE	ME	ΓA	49		17.404	80.914	134.277	0.50	47.30
	256	С	ME	ΓА	49		19.460	82.382	129.018	1.00	45.42
15	257	0	MET	r A	49	•	18.838	82.843	128.049	, 1.00	43.63
	258	N	GLU	JA	50	•	20.510	82.981	129.572	1.00	43.49
	259	CA	GLU	JA	50		21.035	84.231	129.058	1.00	45.80
	260	CB	GLU	JA	50		22.293	84.641	129.829	1.00	48.10
	261	CG	GLU	JA	50		22.023	85.475	131.063	1.00	60.89
20	262	CD	GLU	JA	50	•	21.662	86.904	130.716	1.00	67.75
	263	OE1	GLU	JA	50		22.528	87.602	130.137	1.00	70.54
	264	OE2	GLU	JA	50		20.519	87.322	131.017	1.00	68.32
	265	C	GLU	A.	50	<i>:</i> .	21.392	83.976	127.608	1.00	41.06
	266	0	GLU	Α	50		20.943	84.687	126.715	1.00	40.41
25	26.7	N	ALA	A	51		22.213	82.957	127.389	1.00	37.44
	268	CA	ALA	·Α	51		22.624	82.582	126.044	1.00	35.18
	269	CB	ALA	A	51		23.406	81.295	126.093	1.00	32.93
	270	С	ALA	A	51		21.396	82.403	125.153	1.00	35.31
	271	0	ALA	A	51		21.337	82.946	124.042	1.00	35.44
30	272	N	LEU	A	52		20.409	81.654	125.641	1.00	31.44
	273	CA	LEU	A	52		19.212	81.421	124.844	1.00	37.68
	274	CB	LEU	A	52		18.217	80.499	125.559	1.00	33.73
	275	CG	LEU	A	52		16.936	80.245	124.741	1.00	35.94
	276	CD1	LEU	A	52		17.281	79.633	123.392	1.00	28.69
35	277	CD2	LEU	A	52		16.006	79.313	125.504	1.00	30.87
	278	С	LEU	A	52		18.527	82.725	124.486	1.00	39.83
	279	0	LEU	A	52		18.235	82.966	123.316	1.00	41.72
	280	N	GLN	A	53		18.276	83.569	125.483	1.00	41.29
	281	CA	GLN	A	53		17.627	84.855	125.224	1.00	38.17
40	282	CB	GLN	A	53		17.621	85.736	126.475	1.00	37.50
	283	CG	GLN	A	53		16.823	87.019	126.283	1.00	34.75
	284	CD	GLN	A	53		15.328	86.803	126.441	1.00	41.28
	285	OE1	GLN	A	53		14.826	85.683	126.284	1.00	37.82

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5	333	OD1	ASN	A	60	11.654	87.037	115.132	1.00	47.90
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	. 335	Ċ	ASN	A	60	14.820	87.637	114.230	1.00	48.73
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	337	N	LYS	A	61	15.948	88.300	114.451	1.00	51.94
10	338	CA	LYS	A	61	16.300	89.456	113.652	1.00	54.61
	339	СВ	LYS	A	61	17.292	90.346	114.400	1.00	57.79
	340	CG	LYS	Α	61	16.649	91.109	115.546	1.00	67.28
	341	CD	LYS	A	61	17.530	92.256	116.020	1.00	75.79
	342	CE	LYS	A	61	16.819	93.110	117.071	1.00	78.75
15	343	NZ	LYS	A	61	17.631	94.311	117.454	1.00	81.03
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	346	N	LEU	A	62	17.844	88.186	112.283	1.00	51.98
	347	CA	LEU	A	62	18.472	87.758	111.034	1.00	46.07
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	349	CG	LEU	A	62	20.782	87.190	112.083	1.00	51.21
	350	CD1	LEU	A	62	21.713	86.006	112.341	1.00	53.01
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25	353	Ó	LEU	A	62	17.825	87.046	108.853	1.00	43.64
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	356	С	GLY	A	63	14.873	84.837	109.819	1.00	41.98
	357	0	GLY	Α	63	14.031	84.290	109.090	1.00	37.96
30	358	N	VAL	A	64	15.461	84.195	110.823	1.00	38.22
	359	CA	VAL	A	64	15.152	82.801	111.104	1.00	31.62
	360	СВ	VAL	. A	64	16.059	82.262	112.210	1.00	30.82
	361	CG1	VAL	A	64	15.621	80.858	112.599	1.00	28.03
	362	CG2	VAI	A	64	17.517	82.296	111.736	1.00	22.55
35	363	С	VAI	A	64	13.702	82.684	111.523	1.00	33.79
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	366	CA	LYS	S A	65	11.591	81.461	111.244	1.00	34.02
	367	СВ	LYS	A	65	10.927	80.812	110.024	1.00	32.44
40	368	CG	LYS	A a	65	10.871	81.681	108.764	1.00	42.92
	369	CD	LYS	S A	65	9.713	82.678	108.848	1.00	49.78
	370	CE	LYS		65	9.577	83.506	107.585	1.00	53.74
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•	852	N	THE	. <i>P</i>	127	2.4	19 76.878	3 129.754	1.00	40.32
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	953	CG2	ILE	A'	140		7.543	78.560	116.770	1.00	32.19
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25	955	CD1	ILE	A	140	•	6.059	79.349	114.456	1.00	31.48
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30	960	CB	LEU	A	141	1	1.317	80.451	120.912	1.00	33.19
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	1253	CG1	ILE	Α	179	3.803	58.325	109.923	1.00	21.96
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5	1361	CG	LEU	Α	192	8.851	77.390	108.192	1.00	38.59
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	1363	CD2	LEU	A	192	10.284	77.841	107.959	1.00	30.35
	1364	С	LEU	. A	192	9.245	73.671	109.450	1.00	34.59
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	1369	CG	ARG	A	193	6.056	70.868	110.303	1.00	36.84
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	2004	С	ARG	3 В	37	41.556	60.571	87.386	1.00	34.97
	2005	0	ARG	; в	37	42.055	59.811	86.561	1.00	28.07
5	2006	N	MET	В	38	40.712	61.548	87.057	1.00	35.33
	2007	CA	MET	В	38	40.308	61.818	85.681	1.00	37.27
	2008	СВ	MET	В	38	41.471	62.395	84.874	1.00	38.26
	2009	CG	MET	В	38	41.874	63.792	85.305	1.00	43.26
	2010	SD	MEI	B	38	43.320	64.442	84.413	1.00	50.85
10	2011	CE	MET	В	38	42.639	64.685	82.741	1.00	42.32
	2012	С	MEI	' В	38	39.774	60.581	84.983	1.00	41.75
	2013	0	MET	' В	38	40.097	60.322	83.828	1.00	44.59
	2014	N	GLN	В	39	38.968	59.808	85.694	1.00	38.24
	2015	CA	GLN	В	39	38.368	58.614	85.128	1.00	39.36
15	2016	CB	GLN	В	39.	38.766	57.364	85.937	1.00	40.98
	2017	CG	GLN	ľΒ	39	40.240	56.980	85.829	1.00	43.52
	2018	CD	GLN	В	39	40.588	55.705	86.589	0.50	43.10
•	2019	OE1	GLN	В	39	40.396	55.611	87.803	0.50	39.90
	2020	NE2	GLN	В	39	41.112	54.718	85.870	0.50	44.08
20	2021	С	GLN	В	39	36.858	58.812	85.203	1.00	40.23
	2022	0	GLN	В	39	36.375	59.639	85.969	1.00	34.98
	2023	N	PRO	В	40	36.092	58.072	84.391	1.00	42.21
	2024	CD	PRO	В	40	36.495	57.164	83.304	1.00	48.07
	2025	·CA	PRO	В	40	34.637	58.230	84.443	1.00	45.23
25	2026	CB	PRO	В	40	34.154	57.388	83.258	1.00	47.19
	2027	CG	PRO	В	40	35.238	56.369	83.076	1.00	50.59
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30	2031	CA	ARG	В	41	32.319	58.058	87.504	1.00	49.09
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	2034	CD	ARG		41	29.289	59.748	89.264	1.00	66.85
. -	2035	NE	ARG		41	28.693	59.591	90.588	1.00	67.64
35	2036	CZ	ARG		41	28.506	60.590	91.445	1.00	71.31
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	2038		ARG		41	27.973	60.351		1.00	72.69
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	2043	СВ	VAL		42	31.646	53.729	85.402	1.00	52.94
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	2091	N	MET	В	49	33.744	49.559	95.554	1.00	24.06
5	2092	CA	MET	В	49	33.517	48.144	95.869	1.00	28.88
	2093	CB	MET	В	49	33.130	47.331	94.621	1.00	31.04
	2094	CG	MET	В	49.	31.635	47.133	94.381	1.00	39.52
	2095	SD	MET	В	49	31.234	45.702	93.276	0.50	35.36
	2096	CE	MET	В	49	31.697	46.395	91.762	1.00	37.74
10	2097	С	MET	В	49	34.793	47.551	96.477	1.00	30.80
	2098	0	MET	В	49	34.734	46.752	97.413	1.00	35.99
	2099	N	GLU	В	50	35.950	47.940	95.952	1.00	33.55
	2100	CA	GLU	В	50	37.221	47.426	96.480	1.00	31.25
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15	2102	CG	GLU	В	50	38.554	47.294	94.256	1.00	38.13
	2103	CD	GLU	В	50	38.789	45.789	94.313	1.00	47.32
	2104	OE1	GLU	В	50	39.537	45.337	95.217	1.00	47.00
	2105	OE2	GLU	В	50	38.232	45.061	93.456	1.00	42.37
	2106	C	GLU	В	50	37.384	47.898	97.905	1.00	30.84
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	2109	CA	ALA	В	51	37.286	49.768	99.453	1.00	32.09
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	2111	С	ALA	В	51	36.395	49.008	100.436	1.00	27.96
25	2112	0	ALA	В	51	36.814	48.700	101.548	1.00	30.77
	2113	N	LEU	В	52	35.173	48.686	100.016	1.00	29.85
	2114	CA	LEU	В	52	34.257	47.957	100.891	1.00	25.95
	2115	СВ	LEU	В	52	32.848	47.823	100.274	1.00	26.02
••	2116	CG	LEU	В	52	31.809	47.122	101.177	1.00	26.29
30	2117	CD1	LEU	Ŗ	- 52	31.723	47.839	102.524	1.00	18.74
	2118	CD2	LEU		52	30.432	47.111	100.508	1.00	24.68
	2119	С	LEU		52	34.831	46.581	101.182	1.00	27.37
	2120	0	LEU		52	34.856		102.332	1.00	23.49
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35	2122	CA	GLN		53	35.886	44.574	100.374	1.00	32.31
	2123	CB	GLN		53	36.462	43.988	99.083	1.00	34.86
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40	2126		GLN		53	34.594		99.057	1.00	37.18
40	2127		GLN		53	36.105	40.319		1.00	38.63
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	2301	CG	GL	N B	82		26.328	56.526	87.151	1.00 98.76
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	2303	OE	1 GL	N _. B	82		27.055	58.809	87.041	1.00 98.73
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	2312	OE1	LGL	ЈΒ	83		21.267	58.612	89.362	0.00 99.48
	2313	OE2	GL(Ј В	83		21.225	56.495	.89.938	0.00 99.48
	2314	С	GLU	ј В	83		21.407	53.252	87.498	1.00 99.34
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	2316	N	VAI	В	84		20.163	52.920	87.156	1.00100.00
	2317	CA	VÄL	В	84		19.747	51.521	86.978	1.00100.00
	2318	СВ	VAL	В	84	,	18.263	51.420	86.471	1.00100.00
	2319	CG1	VAL	В	84	•	17.268	51.796	87.589	1.00 99.23
25	2320	CG2	VAL	В	84		18.076	52.328	85.269	1.00100.00
	2321	С	VAL	В	84		20.645	50.721	86.012	1.00100.00
	2322	0	VAL	В	84		20.416	49.518	85.793	1.00100.00
	2323	N	LYS	В	85		21.667	51.379	85.454	1.00 96.27
	2324	CA	LYS	В	85		22.564	50.722	84.514	1.00 91.89
30	2325	СВ	LYS	В	85		23.052	51.715	83.457	1.00 92.14
	2326	CG	LYS	В	85		23.655	51.051	82.243	0.00 91.98
	2327	CD	LYS	В	85		24.401	52.034	81.339	0.00 91.89
	2328	CE	LYS	В	85		25.031	51.302	80.154	0.00 91.77
	2329	NZ	LYS	В	85		25.878	52.209	79.338	0.00 91.53
35	2330	С	LYS	В	85		23.759	50.084	85.215	1.00 90.19
	2331	0	LYS	В	85		23.699	48.911	85.616	1.00 86.89
	2332	N	PHE	В	86		24.837	50.852	85.377	1.00 89.52
	2333	CA	PHE	В	86		26.035	50.321	86.019	1.00 88.74
	2334	CB	PHE	В	86		27.275	51.138	85.641	1.00 92.15
40	2335	CG	PHE	В	86		27.777	50.850	84.253	1.00 98.73
	2336	CD1	PHE	В	86		27.403	51.658	83.178	1.00 99.74
	2337	CD2	PHE	В	86		28.594	49.744	84.009	1.00100.00
	2338	CE1	PHE	В	86		27.834	51.370	81.872	1.00100.00

	2339) CE	22 PH	IE E	86	29.031	49.442	82.709	1.00	100.00
	2340) Cz	Z PH	E E	86	28.649	50.259	81.637	1.00	100.00
	2341	L C	PH	E E	86	25.988	50.127	87.534	1.00	85.29
	2342	2 0	PH	E	86	26.644	49.219	88.051	1.00	84.94
5	2343	B N	IL	E B	87	25.232	50.955	88.252	1.00	80.15
	2344	CA	IL.	E B	87	25.134	50.789	89.701	1.00	75.10
	2345	CE	IL.	E B	87	24.651	52.075	90.395		73.06
	2346	CG	2 IL	Е В	87	24.352	51.792	91.873		72.58
	2347	CG	1 IL	ΕВ	87	25.724	53.160	90.271		
10	2348	CD	1 IL	Е В	87	25.436	54.404	91.090	1.00	70.71
	2349	С	IL	Е В	87	24.199	49.632	90.084		72.87
	2350	0	IL	ΕВ	87	24.378	49.010	91.132		73.21
	2351	N	ME	т в	88	23.203	49.343	89.250		70.19
	2352	CA	ME	т в	88	22.297	48.233	89.537		68.05
15	2353	СВ	ME'	г в	88	20.942	48.432	88.854		68.28
	2354	CG	ME:	гв	88	20.012	49.364	89.626		66.92
	2355	SD	ME	г в	88	19.619	48.738	91.273		59.10
	2356	CE	MES	г в	88	18.028	49.538	91.593		67.20
	2357	С	MET	г в	88	22.913	46.913	89.101	1.00	66.04
20	2358	0	MET	B	88	22.416	45.844	89.444	1.00	68.71
	2359	N	ASN	1 B	89	24.002	46.997	88.347		64.44
	2360	CA	ASN	В	89	24.719	45.817	87.884	1.00	62.80
	2361	CB	ASN	I B	89	25.225	46.019	86.456	1.00	70.00
	2362	CG	ASN	В	89	24.345	45.342	85.425	1.00	80.14
25	2363		ASN		89	23.142	45.618	85.326	1.00	85.25
٠.,	2364		ASN		89	24.942	44.444	84.647	1.00	83.00
	2365	С	ASN	В	89	25.905	45.523	88.798	1.00	60.13
	2366	0	ASN		89	26.618	44.537	88.592	1.00	57.81
20	2367	N	LEU		90	26.121	46.379	89.800	1.00	53.28
30	2368	CA	LEU		90	27.229	46.185	90.743	1.00	50.44
	2369	CB	LEU		90	27.522	47.473	91.534	1.00	48.07
	2370	CG	LEU		90	28.133	48.680	90.792	1.00	51.30
	2371		LEU		90	28.202	49.877	91.723	1.00	47.19
25	2372		LEU		90	29.517	48.346	90.261	1.00	47.85
35	2373	C	LEU		90	26.941	45.040	91.710	1.00	46.83
•	2374	0	LEU		90	27.834	44.256	92.032	1.00	44.52
	2375	N	PRO		91	25.691	44.929	92.196	1.00	46.91
	2376	CD	PRO		91	24.537	45.840	92.097	1.00	45.81
40	2377	CA	PRO		91	25.400	43.834	93.121	1.00	44.29
40	2378	CB	PRO		91	23.910	43.997	93.377	1.00	47.92
	2379	CG	PRO		91		45.491	93.342	1.00	15.72
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	2381	0	PRO	В	91	26.161	41.555	93.073	1.00	12.25

	2382	2 N	VA	T E	3 92	25.544	42.504	91.126	1.00 42.78
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	2384	CE	VA	LE	92	25.253	41.425		
	2385	co	1 VA	L.E	92	25.575	40.184		
5	2386	ce	2 VA	L B	92	23.734	41.642	88.994	
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	2388	0	VA	L B	92	27.836	40.015	90.530	1.00 50.14
	2389	N	GL	UВ	93	28.077	42.193	90.001	1.00 46.79
	2390	CA	GL	U B	93	29.534	42.127	89.921	1.00 46.04
. 10	2391	СВ	GL	UВ	93	30.099	43.477	89.486	1.00 54.15
	2392	CG	GL	UВ	93	31.616	43.579	89.523	1.00 62.65
	2393	CD	GL	UВ	93	32.180	44.336	88.322	1.00 72.41
	2394	OE	1 GL	UВ	93	31.566	45.346	87.889	1.00 69.66
	2395	OE	2 GL	UВ	93	33.248	43.916	87.817	1.00 78.42
15	2396		GL	U B	93	30.087	41.750	91.278	1.00 42.44
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00	2400	СВ		ΞВ	94	28.867	42.740	94.633	1.00 39.94
20	2401	CG		ΞВ	94	29.188	42.577	96.101	1.00 38.23
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	2403	CD2			94	28.289	41.927	96.948	1.00 37.14
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23.	2406	CZ	PHE		94	29.731	42.349	98.839	1.00 31.62
	2407 2408	С	PHE		94	29.768	40.497	93.946	1.00 38.73
	2409	O N	PHE		94	30.760	39.896	94.352	1.00 41.46
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30	2411	CB	TYR		95 95	28.394	38.466	93.905	1.00 44.84
	2412	CG	TYR		95	26.978 26.728	38.053	93.482	1.00 46.83
	2413		TYR		95	26.525	36.571 36.019	93.658	
	2414		TYR		95	26.371	34.642	94.930	
	2415		TYR		95	26.763	35.706	95.103 92.563	1.00 50.61
35	2416		TYR		95	26.610	34.322	92.728	1.00 53.25 1.00 53.76
	2417	CZ	TYR		95	26.417	33.799	93.998	1.00 53.78
	2418	ОН	TYR		95	26.281	32.433	94.155	1.00 55.30
	2419	С	TYR		95	29.382	37.601	93.146	1.00 47.75
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	5435	CG	ARG C	244	31.099	38.172	163.205	1.00	72.92
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5	5903	CD	1 PH	E D	72	23.268	58.381 170.662	1.00 96.57
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	5905	CE	1 PH	E D	72	22.924	57.160 171.259	1.00 95.11
	5906	CE	2 PH	E D	72	23.785	57.962 173.369	1.00 97.98
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	5914	С	SEE	R D	73	24.504	56.405 167.520	1.00 86.94
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20	5918	CB	THE	R D	78	22.680	55.101 177.973	0.30 93.10
	5919	OG1	L THE	R D	78	22.345	53.792 178.446	0.30 92.02
	5920	CG2	THF	D	78	23.118	55.013 176.519	0.30 91.79
	5921	С	THE	D	78	23.285	55.910 180.258	0.30 95.37
	5922	0	THR	D	78	22.582	55.064 180.811	0.30 95.17
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	5926	CG	ARG	D	79	24.599	55.479 183.150	0.30 98.06
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	5929	CZ	ARG	D	79	26.676	53.018 185.050	0.30 96.66
	5930	NH1	ARG	D	79	27.219	53.683 186.061	0.30 95.97
	5931	NH2	ARG	D	79	26.912	51.721 184.911	0.30 96.02
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40	5938	CG	PRO	D	80	19.753	59.468 183.940	1.00 99.83
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5	6029	СВ	PRO	D	91	26.725	72.901	174.004	1.00	39.04
	6030	CG	PRO	D	91	26.470	71.438	173.905	1.00	35.14
	6031	Ċ	PRO	D	91	28.673	74.218	174.935	1.00	39.02
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	6033	N	VAL	D	92	28.497	74.296	176.244	1.00	38.20
10	6034	CA	VAL	D	92	28.906	75.491	176.950	1.00	37.45
	6035	СВ	VAL	D	92	28.434	75.451	178.425	1.00	37.04
	6036	CG1	VAL	D	92	28.359	76.866	178.988	1.00	30.49
	6037	CG2	VAL	D	92	27.076	74.762	178.508	1.00	39.79
	6038	С	VAL	D	92	30.436	75.590	176.882	1.00	37,.83
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	6042	CB	GLU	D	93	33.115	73.070	177.612	1.00	49.36
	6043	CG	GLU	D	93	33.334	72.914	179.112	1.00	60.54
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	6045	OE1	GLU	D	93	34.868	71.080	178.950	1.00	66.48
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	6047	С	GLU	D	. 93	33.109	74.718	175.745	1.00	43.85
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25	6049	N	PHE	D	94	32.432	74.147	174.757	1.00	40.25
	6050	CA	PHE	D	94	32.820	74.354	173.377	1.00	41.92
	6051	CB	PHE	D	94	31.875	73.601	172.437	1.00	44.47
	6052	CG	PHE	D	94	32.299	73.646	171.005	1.00	40.18
	6053	CD1	PHE	D	94	33.453	72.967	170.588	1.00	38.25
30	6054	CD2	PHE	D	94	31.592	74.411	170.086	1.00	39.02
	6055	CE1	PHE	D	94	33.900	73.056	169.273	1.00	32.89
	6056	CE2	PHE	D	94	32.033	74.507	168.767	1.00	39.32
	6057	CZ	PHE	D	94	33.193	73.828	168.364	1.00	25.20
	6058	С	PHE	D	94	32.760	75.840	173.068	1.00	42.55
35	6059	0	PHE		94	33.710	76.408	172.527	1.00	47.20
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	6063	CG	TYR		95	29.886	79.850	173.641	1.00	45.63
40	6064		TYR	D	95	29.873	80.562	172.434	1.00	47.08
	6065	CE1	TYR	D	95	29.738	81.948	172.413	1.00	45.11
	6066	CD2	TYR	D	95			174.824	1.00	49.03
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	6458	СВ	ALA	D	144	23.236	66.765	163.475	1.00	17.78
	6459	С	ALA	D	144	23.023	67.567	165.843	1.00	21.99
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	6464	CG	LEU	D	145	23.785	69.589	168.814	1.00	38.09
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	6862	0	PRO	D	195		26.147	64.246	150.004	1.00	27.41
25	6863	N	ASP	D	196		27.988	65.498	150.072	1.00	21.62
	6864	CA	ASP				28.578	64.775	148.956	1.00	20.52
	6865	СВ	ASP	D	196		29.644	65.623	148.269	1.00	27.06
	6866	CG	ASP				29.073	66.868	147.663	1.00	26.11
00	6867		ASP				29.120		148.321	1.00	21.26
30	6868		ASP				28.552		146.531		36.91
	6869	С	ASP				29.231		149.480		
	6870	0	ASP				29.271		148.792		21.30
	6871	N	LEU				29.731		150.712		19.60
25	6872	CA	LEU				30.432		151.354		20.66
35	6873	CB	LEU				31.955		151.338		18.94
	6874	CG	LEU				32.863		152.156		23.54
	6875	CD1					32.949		151.498		16.11
	6876		LEU				34.245		152.237		16.20
40	6877	С	LEU				29.976		152.803		17.57
40	6878	0	LEU				29.797		153.453		18.10
	6879	N	ILE				29.774		153.304		13.50
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	6925	СВ	GLU	D	204		29.550	52.207	163.360	1.00	38.54
	6926	CG	GLU	D	204		, 29.673,	52.127	164.861	1.00	50.00
	6927	CD	GLU	D	204		29.435	50.719	165.371	1.00	55.94
	6928	OE1	GLU	D	204		28.454	50.087	164.919	1.00	60.50
5	6929	OE2	GĽΰ	D	204		30.223	50.241	166.219	1.00	60.12
	6930	С	GLU	D	204 .	•	29.914	51.114	161.148	1.00	28.99
	6931	0	GLU	D	204		30.197	52.067	160.436	1.00	33.53
-	6932	N	LEU	· D	205		29.281	50.045	160.688	1.00	27.12
	6933	CA	LEU	D	205		28.851	49.962	159.302	1.00	28.21
10	6934	СВ	LEU	. D	205		29.314	48.639	158.681	1.00	34.86
	6935	CG	LEU	D	205		30.613	48.543	157.849	1.00	40.22
	6936	CD1	LEU	D	205		.30.273	48.538	156.357	1.00	39.68
	6937	CD2	LEU	D	205		31.564	49.692	158.172	1.00	37.50
	6938	С	LEU	D	205		27.339	50.074	159.252	1.00	27.93
15	6939	0	LEU	· D	205		26.646	49.145	158.864	1.00	33.73
	6940	N	ARG	D	206		26.828	51.216	159.681	1.00	29.79
	6941	CA	ARG	D	206		25.398	51.467	159.673	1.00	30.19
	6942	CB	ARG	D	206		24.767	50.931	160.950	1.00	30.10
	6943	CG	ARG	D	206		25.227	51.612	162.198	1.00	34.91
20	6944	CD	ARG	D	206		24.366	51.211	163.353	1.00	34.39
	6945	NE	ARG	D	20.6		24.790	49.943	163.901	1.00	45.41
	6946	CZ	ARG	D	206		25.557	49.822	164.977	1.00	52.92
	6947	NH1	ARG	D	206		25.971	50.908	165.618	1.00	54.52
	6948	NH2	ARG	D	206		25.906	48.614	165.408	1.00	56.84
25	6949	С	ARG	D	206	•	25.197	52.973	159.542	1.00	33.05
	6950	0	ARG	D	206		26.104	53.761	159.827	1.00	33.47
	6951	N	LEU	D	207		23.999	53.385	159.158	1.00	35.91
	6952	CA	LEU	D	207		23.713	54.803	158.913	1.00	37.61
	6953	CB	LEU				22.821	54.878	157.659	1.00	45.71
30	6954	.CG	LEU	D	207		22.238	53.504	157.242	1.00	41.56
	6955	CD1	LEU	D	207		21.609	52.854	158.467	1.00	37.60
	6956	CD2	LEU	D	207		21.181	53.642	156.104	1.00	39.02
	6957	С	LEU	D	207		23.123		160.049	1.00	37.51
	6958	0	LEU	D	207		23.120		159.967	1.00	38.35
35	6959	N	SER	D	208		22.628	55.017	161.092	1.00	24.15
	6960	CA	SER	D	208		22.028	55.671	162.253	1.00	20.91
	6961	CB	SER	D	208		23.115	56.049	163.246	1.00	18.47
	6962	OG	SER	D	208		23.784	54.888	163.659	1.00	21.46
	6963	С	SER	D	208		21.070	56.855	162.108	1.00	22.71
40	6964	0	SER	D	208		21.095	57.784	162.916	1.00	22.82
	6965	N	ASN				20.222	56.835	161.094	1.00	21.42
	6966	CA	ASN	D	209		19.231	57.893	160.961	1.00	17.48
	6967	CB	ASN	D	209		18.299	57.809	162.188	1.00	16.20

	6968	CG	ASN	D	209	16.963	58.515	161.987	1.00	19.86
	6969	OD1	ASN	D	209	16.486	58.700	160.868	1.00	14.67
	6970	ND2	ASN	D	209	16.347	58.895	163.092	1.00	17.14
	6971	С	ASN	D	209	19.852	59.296	160.824	1.00	17.04
5	6972	0	ASN	D	209	19.303	60.280	161.302	1.00	14.34
	6973	N	PHE	D	210	21.001	59.368	160.170	1.00	18.04
	6974	CA	PHE	D	210	21.684	60.638	159.921	1.00	16.36
	6975	СВ	PHE	D	210	23.180	60.484	160.149	1.00	19.10
	6976	CG	PHE	D	210	23.956	61.764	159.969	1.00	21.10
10	6977	CD1	PHE	D	210	23.655	62.874	160.727	1.00	14.31
•	6978	CD2	PHE	D	210	24.995	61.840	159.046	1.00	19.80
	6979	CE1	PHE	D	210	24.374	64.059	160.577	1.00	19.27
	6980	CE2	PHE	D	210	25.729	63.025	158.885	1.00	23.51
	6981	CZ	PHE	D	210	25.417	64.131	159.649	1.00	15.26
15	6982	С	PHE	D	210	21.446	61.061	158.470	1.00	15.01
	6983	0	PHE	D	210	21.847	60.364	157.552	1.00	18.32
	6984	N	LEU	D	211	20.776	62.193	158.282	1.00	17.17
	6985	CA	LEU	D	211	20.481	62.733	156.952	1.00	15.46
	6986	CB	LEU	D	211	21.732	63.443	156.385	1.00	12.81
20	6987	CG	LEU	D	211	22.345	64.548	157.290	1.00	16.60
	6988	CD1	LEU	D	211	23.595	65.129	156.641	1.00	18.96
	6989	CD2	LEU	D	211	21.342	65.654	157.563	1.00	8.25
	6990	С	LEU	D	211	19.931	61.734	155.924	1.00	18.70
	6991	0	LEU	D	211	20.428	61.659	154.805	1.00	18.32
25	6992	N	PRO	D	212	18.889	60.955	156.289	1.00	17.80
•	6993	CD	PRO	D	212	18.225	60.881	157.595	1.00	17.20
	6994	CA	PRO	D	212	18.294	59.979	155.364	1.00	18.97
	6995	CB	PRO	D	212	17.088	59.420	156.148	1.00	19.76
	6996	CG	PRO	D	212	16.818	60.432	157.181	1.00	24.29
30	6997	С	PRO	D	212	17.892	60.573	154.015	1.00	15.44
	6998	0	PRO	D	212	18.221	60.033	152.945	1.00	13.00
١	6999	N	TRP	D	213	17.182	61.681	154.053	1.00	12.04
•	7000	CA	TRP	D	213	16.798	62.323	152.797	1.00	15.79
	7001	СВ	TRP	D	213	15.773	63.416	153.060	1.00	12.12
35	7002	CG	TRP	D	213	15.361	64.156	151.845	1.00	16.46
	7003		TRP			14.125	64.013	151.149	1.00	19.97
	7004	CE2	TRP	D	213	14.126	64.962	150.091	1.00	20.58
	7005		TRP			13.012	63.182	151.315	1.00	14.88
	7006		TRP			16.056	65.151	151.198	1.00	15.78
40	7007		TRP			15.317	65.641	150.148	1.00	20.92
	7008	CZ2	TRP	D	213	13.059	65.096	149.210	1.00	20.31
	7009	CZ3	TRP	D	213	11.943	63.318	150.435	1.00	25.52
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	7011	С	TRP I	213	17.990	62.939	152.047	1.00	16.94
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	7013	N	GLN I	214	18.644	63.895	152.702	1.00	15.86
	7014	CA	GLN I	214	19.784	64.618	152.133	1.00	17.05
5	7015	СВ	GLN I	214	20.291	65.666	153.133	1.00	14.93
	7016	CG	GLN I	214	19.230	66.625	153.701	1.00	13.05
	7017	CD	GLN I	214	18.662	66.150	155.059	1.00	16.53
	7018	OE1	GLN I	214	18.228	66.953	155.894	1.00	18.57
	7019	NE2	GLN I	214	18.653	64.851	155.265	1.00	9.63
10	7020	С	GLN I	214	20.959	63.727	151.677	1.00	16.49
	7021	0	GLN [214	21.602	64.030	150.681	1.00	17.95
	7022	Ŋ	GLY I	215	21.212	62.627	152.388	1.00	19.08
	7023	CA	GLY I	215	22.299	61.719	152.040	1.00	13.31
	7024	С	GLY [215	21.923	60.554	151.138	1.00	17.46
15	7025	0	GLY I	215	22.719	59.658	150.946	1.00	18.16
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•	7027	CA	ALA [216			149.683	1.00	22.36
	7028	СВ	ALA [216			149.004		23.76
••	7029	C	ALA D				148.612		21.72
20	7030	0	ALA C				148.282		22.39
	7031	N	TYR D				148.064		18.33
	7032	CA	TYR D				147.040		19.11
•	7033	CB	TYR D			•	145.747		21.81
25	7034	CG	TYR D				145.118		22.69
25	7035		TYR D				145.396		25.39
	7036		TYR D				144.778		25.57
	7037		TYR D		21.159		144.213		22.79
	7038		TYR D				143.588		23.27
30	7039	CZ OH	TYR D				143.874		
50	7040 7041	С	TYR D		17.739		143.211		35.64
	7041	0	TYR D				147.456		
	7042	N	SER D		25.361 24.706		146.638 148.708		23.26
	7043	CA	SER D		26.066		149.147		21.01 19.51
35	7045	CB	SER D		26.065		150.604		19.16
	7046	OG	SER D		25.191		150.786		23.90
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	7048	0	SER D		26.631		149.163		20.49
	7049	N	GLU D		28.304		148.856		24.47
40	7050	CA	GLU D		29.354				19.81
- •	7051	CB	GLU D		30.671		148.295		26.14
	7052	CG	GLU D				146.795		29.57
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			J_J D		55.472	55.059	T40.07T	1.00	20.34

	7054	OE1	. GLU I	219	31.111	57.021	146.460	1.00	31.78
	7055		GLU I		29.707		145.066		41.97
	7056	C		219	29.538		150.324		17.55
•	7057	0		219	29.529		151.139		17.42
5	7058	N		o [.] 220	29.676		150.684		18.74
	7059	CA		220			152.087		22.81
	7060	СВ	LEU I	'			152.525		13.34
	7061	CG	LEU I		27.379		152.291		22.63
	7062	CD1	LEU I	220 -	26.553		152.648		19.93
10	7063	CD2	LEU I	220	26.933	57.072	153.102	1	14.34
	7064	С	LEU I	220	31.298	56.239	152.317	1.00	28.88
	7065	0	LEU I	220	31.900	55.551	151.482	1.00	27.20
	7066	N	TYR I	221	31.845	56.634	153.457	1.00	24.42
	7067	CA	TYR I	221	33.199	56.276	153.803	1.00	28.17
15	7068	СВ	TYR I	221	34.122	57.473	153.571	1.00	29.00
	7069	CG	TYR I	221	35.531	57.233	154.018	1.00	29.40
	7070	CD1	TYR I	221	36.424	56.494	153,239	1.00	29.58
	7071	CE1	TYR D	221	37.724	56.267	153.677	1.00	27.31
	7072	CD2	TYR I	221	35.971	57.728	155.232	1.00	26.93
20	7073	CE2	TYR I	221	37.251	57.510	155.672	1.00	24.96
	7074	CZ	TYR D	221	38.124	56.787	154.908	1.00	28.52
	7075	ОН	TYR D	221	39.395	56.587	155.399	1.00	34.32
	7076	С	TYR Ç	221	33.213	55.855	155.265	1.00	30.35
	7077	0	TYR D	221	32.855	56.631	156.155	1.00	32.66
25	7078	N	PHE D	222	33.599	54.607	155.495	1.00	31.08
	7079	CA	PHE D	222	33.673	54.040	156.834	1.00	28.64
	7080	СВ	PHE D		32.930		156.887	1.00	25.60
	7081	CG	PHE D		31.496	52.785	156.452	1.00	21.34
00	7082		PHE D		31.155		155.109	1.00	18.25
30	7083		PHE D		30.495		157.381		21.90
	7084				29.829	52.804	154.696	1.00	24.31
	7085		PHE D		29.164		156.980	1.00	18.83
	7086	CZ	PHE D		28.832		155.635	1.00	22.46
25	7087	С	PHE D					1.00	28.93
35	7088	0	PHE D					1.00	32.66
	7089	N	THR D				158.465		25.87
	7090	CA	THR D		36.802		158.961	1.00	26.29
	7091	CB	THR D				158.883		30.16
40	7092		THR D					1.00	29.78
40	7093		THR D				159.756	1.00	
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	7095	0	THR D					1.00	
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35	7260	СВ	ARG	D	244	39.581	56.855	144.592	1.00	58.07
	7261	CG	ARG	D	244	41.077	56.769	144.384	1.00	66.11
	7262	CD	ARG	D	244	41.807	57.981	144.923	1.00	73.72
	7263	NE	ARG	D	244	43.230	57.696	145.119	1.00	81.74
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                       12
                                        63.433 156.365
                                                         1.00 18.54
35
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           OH2 WAT W
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                                        67.674 105.333
                                                         1.00 44.98
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           OH2 WAT W
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                                        86.622 162.346
                                                         1.00 18.68
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           OH2 WAT W
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                                        36.086 111.611
                                                         1.00 20.08
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           OH2 WAT W
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                                        64.439 109.100
                                                         1.00 29.10
           OH2 WAT W
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                                        40.959 124.848
                                                         1.00 65.65
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           OH2 WAT W
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           OH2 WAT W
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                                        55.192 170.279
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                                        35.046 152.724
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           OH2 WAT W
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                       21
                               15.333
                                                         1.00 28.72
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	7312	ОН2	RW S	r W	22	30.959	61.833 94.884	1.00 26.91
	7313	ОН2	raw s	. M	23	13.805	60.126 163.832	1.00 30.48
	7314	OH2	RAW S	W	24	27.234	69.610 148.193	1.00 22.34
	7315	ОН2	LAW S	r W	25	18.824	60.189 114.266	1.00 23.07
5	7316	ОН2	raw s	W	26	41.077	49.283 99.183	1.00 37.57
	7317	OH2	LAW S	W	27	10.572	28.703 137.018	1.00 37.26
	7318	OH2	RAW	W	28	16.340	75.164 175.623	1.00 27.57
	7319	OH2	RAW	W	29	23.460	60.770 117.115	1.00 26.41
	7320	OH2	RAW	W	30	40.206	58.426 156.934	1.00 32.69
10	7321	OH2	RAW	W	31	6.625	51.188 155.796	1.00 23.16
	7322	OH2	raw :	W	32	45.626	67.086 162.002	1.00 34.83
	7323	OH2	raw :	W	33	10.396	75.275 139.683	1.00 44.91
	7324	OH2	raw :	W	34	-0.601	31.861 146.272	1.00 24.79
	7325	OH2	WAT	W	35	17.494	70.622 152.608	1.00 24.54
15	7326	OH2	WAT	W	36	40.844	64.399 177.253	1.00 38.86
	7327	OH2	WAT	W	37	9.317	76.714 155.588	1.00 44.72
	7328	ОН2	TAW	W	38	27.274	48.442 122.282	1.00 49.70
	7329	ОН2	TAW	W	39	16.004	37.400 99.199	100 43.82
	7330	ОН2	WAT	W	40	12.464	57.862 103.307	1.00 25.85
20	7331	OH2	WAT	W	41	16.000	50.457 119.288	1.00 41.83
	7332	OH2	WAT	W	42	11.536	62.676 115.517	1.00 21.38
	7333	OH2	WAT	W	43	29.945	32.976 146.925	1.00 40.38
	7334	OH2	WAT	W	44	34.140	42.113 149.283	1.00 42.33
~ ~	7335		WAT		45	7.925	76.405 126.399	1.00 39.14
25	7336		WAT		46	18.170	61.725 111.986	1.00 20.89
	7337		WAT		47	30.755	77.804 153.505	1.00 19.49
	7338		TAW		48	41.754	57.323 159.509	1.00 50.17
	7339				49	0.432	34.807 151.800	1.00 32.45
20	7340		TAW		50	7.115	42.218 141.155	1.00 44.48
30	7341		TAW		51	41.819	59.321 114.776	
	7342		TAW		52		64.241 166.321	
	7343		TAW		53	-2.402	•	
	7344		WAT		54	30.018	57.511 96.725	
35	7345		WAT		55	25.854		
<i>.</i>	7346		WAT		56	29.404		1.00 39.21
	7347		WAT WAT		57 50	7.137	64.606 107.354	1.00 35.06
•	7348 7349				58	30.727	50.059 87.237	1.00 54.96
			WAT		59 60	19.413		1.00 35.31
40	7350 7351		TAW TAW		60		88.427 157.351	1.00 26.19
70	7351		WAT		61 62	27.419	47.353 95.987	1.00 57.79
	7352		WAT		63	30.203	48.522 96.797	1.00 54.20
	7354		WAT		64		84.485 164.897	1.00 41.99
	1334	Onz	AALT	VV	04	22.158	87.861 165.582	1.00 33.54

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            OH2 WAT W
                        66
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                        67
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	7398	OH2	WAT	W	108	1	3.929	50.26	4 161.908	1.00	38.42
	7399	ОН2	WAT	W	109		7.928	47.57	3 126.723	1.00	61.79
	7400	ОН2	WAT	W	110	1	6.984	39.54	7 84.255	1.00	46.21
	7401	OH2	WAT	W	111	1	5.832	47.36	6 114.819	1.00	33.95
5	7402	ОН2	TAW	W	112	1	3.984	73.45	1 167.234	1.00	54.71
	7403	OH2	TAW	W	113		9.368	43.08	92.878	1.00	24.54
	7404	OH2	WAT	W	114	_	3.176	65.32	8 167.249	1.00	54.79
	7405	OH2	TAW	W	115	1	0.815	55.60	1 163.806	1.00	36.83
	7406	OH2	WAT	W	116	1	5.643	54.41	5 93.626	1.00	56.57
10	7407	OH2	WAT	W	117	1	8.184	73.66	3 165.116	1.00	34.52
	7408	OH2	WAT	W	118		5.305	83.28	3 114.524	1.00	25.41
	7409	OH2	WAT	W	119	3	2.518	33.65	7 139.051	1.00	49.90
	7410	OH2	WAT	W	120	. 1	7.065	74.47	1 161.007	1.00	49.07
	7411	OH2	WAT	W	121	3	3.595	77.51	2 125.281	1.00	50.88
15	7412	OH2	WAT	W	122	1	7.588	81.10	3 156.085	1.00	50.84
	7413	OH2	WAT	W	123	4	1.500	66.05	4 175.536	1.00	56.58
	7414	OH2	WAT	W	124		5.172	72.06	8 141.250	1.00	41.51
	7415	OH2	WAT	W	125	. 2	1.568	76.16	6 143.755	1.00	73.77
	7416	OH2	WAT	W	126		9.185	62.73	5 142.948	1.00	41.89
20	7417	OH2	WAT	W	127	3	4.832	65.83	7 107.513	1.00	45.85
	7418	ОН2	TAW	W	128		7.851	35.88	1 155.165	1.00	39.11
	7419	OH2	WAT	W	129	2	2.684	74.04	2 102.458	1.00	46.57
	7420	OH2	WAT	W	130	2	7.459	69.12	5 104.582	1.00	38.96
	7421	OH2	WAT	W	131	• -	4.070	57.06	5 158.275	1.00	52.53
25	7422	OH2	TAW	W	132	. 2	8.752	47.21	86.649	1.00	58.61
·	7423	OH2	WAT	W	133	2	4.922	79.09	2 178.645	1.00	45.28
	7424	OH2	TAW	W	134	3	3.981	87.88	5 155.674	1.00	30.59
	7425	OH2	TAW	W	135	1	4.099		3 139.548	1.00	46.13
•	7426	OH2				3	7.470	57.62	5 139.398	1.00	56.59
30	7427		WAT				8.013		9 158.862		44.49
	7428		WAT				2.958		3 168.772	1.00	53.20
	7429		TAW				3.235		7 144.157	1.00	65.83
	7430		WAT				0.003		1 109.124		49.61
25	7431		TAW				1.759		9 106.675		39.16
35	7432		WAT				8.901		162.622		56.01
	7433		TAW				6.104		159.620		23.82
	7434		WAT				1.060		3 103.443		39.92
	7435		TAW				8.774		155.516		51.22
40	7436		TAW				9.091		124.194		54.32
40	7437		WAT				5.574	36.847			35.16
	7438		TAW						2 140.583		66.74
	7439								100.220		41.74
	7440	OH2	WAT	W	150	13	3.217	56.304	100.592	1.00	48.44

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35.169 93.881
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                                      45.202 104.320
                                                      1.00 28.71
     7516
           OH2 WAT W 226
                              8.591
                                      65.733 103.272
                                                      1.00 57.01
     7517
           OH2 WAT W 227
                              30.428
                                      51.766 96.862
                                                      1.00 50.60
35
     7518
           OH2 WAT W 228
                              44.492
                                      73.582 159.662
                                                     1.00 43.18
     7519
           OH2 WAT W 229
                              32.532 65.642 171.323
                                                     1.00 47.34
     7520
           OH2 WAT W 230
                              19.465
                                      41.490 138.172
                                                     1.00 54.20
     7521
           OH2 WAT W 231
                              13.642
                                      56.805 126.904
                                                     1.00 40.69
     7522
           OH2 WAT W 232
                              44.304
                                      58.292 163.071
                                                     1.00 49.23
40
     7523
           OH2 WAT W 233
                                      41.717 159.137
                              33.111
                                                     1.00 54.29
     7524
          OH2 WAT W 234
                                      79.626 183.577
                              19.277
                                                     1.00 34.10
     7525
           OH2 WAT W 235
                              34.633
                                      63.753 113.280
                                                     1.00 47.87
     7526
           OH2 WAT W 236
                              22.154
                                      58.890 155.143
                                                     1.00 34.96
```

	7527	OH2 WA	T TAT	227	41 806	55.096 166.377	1.00 34.24
	7527 7528	OH2 WA			21.432	37.843 88.704	
	7529	OH2 WA			34.643	72.266 132.775	1.00 54.92
	7530	OH2 WA			35.338	85.572 172.058	
5	7531	OH2 WA	r W	241	16.256	49.306 116.927	1.00 31.04
	7532	OH2 WA			41.709	64.265 169.935	1.00 38.19
	7533	OH2 WA			28.757	83.671 179.021	
	7534	OH2 WA			38.413	67.817 108.876	
	7535	OH2 WA			20.663	64.332 111.428	1.00 38.62
10	7536	OH2 WA			43.979	55.862 105.039	1.00 50.24
	7537	OH2 WA	r w	247	43.780	71.588 161.864	1.00 34.98
	7538	OH2 WA	r w	248	11.436	89.641 129.977	1.00 42.00
	7539	OH2 WA	r w	249	41.365	43.999 104.687	1.00 30.91
	7540	OH2 WA	r w	250	15.533	65.748 164.990	1.00 39.00
15	7541	OH2 WA	r W	251	42.846	65.656 89.632	1.00 43.71
	7542	OH2 WA	r W	252	21.227	58.593 112.048	1.00 35.62
٠.	7543	OH2 WA	r w	253	5.127	90.024 111.033	1.00 52.52
	7544	OH2 WA	r w	254	35.042	73.905 117.216	1.00 44.07
	7545	OH2 WA	r w	255	18.017	23.723 142.245	1.00 67.41
20	7546	OH2 WAS	r W	256	-1.547	33.928 137.556	1.00 47.00
	7547	OH2 WAS	r W	257	10.061	75.671 157.442	1.00 55.48
	7548	OH2 WAS	r W	258	7.530	43.022 110.558	1.00 55.53
	7549	OH2 WA	r W	259	26.307	46.356 121.321	1.00 52.54
	7550	OH2 WAS	r W	260	37.686	38.689 95.823	1.00 44.59
25	7551	OH2 WA	W	261	25.245	31.371 90.883	1.00 53.17
	7552	OH2 WA	W	262	-4.652	34.436 142.767	1.00 43.66
	7553	OH2 WAT	W	263	40.945	75.530 172.545	1.00 55.53
	7554	OH2 WAT			-0.740	50.671 134.055	1.00 53.15
	7555	OH2 WAT	W	265	11.352	89.628 133.396	1.00 49.20
30	7556	OH2 WAT	W	266	37.290	34.588 109.736	1.00 50.49
	7557	OH2 WAT	· W	267	40.825	37.013 101.903	1.00 49.39
	7558	OH2 WAT			18.719	39.974 104.690	
	7559	OH2 WAT			0.643	78.513 120.772	1.00 40.99
٥.5	7560	OH2 WAT			-4.940	•	
35	7561	OH2 WAT			13.901		1.00 60.43
	7562	OH2 WAT			40.786	77.684 170.897	1.00 53.15
	7563	OH2 WAT			37.863	51.299 89.365	1.00 43.90
	7564	OH2 WAT			30.617		1.00 42.40
40	7565	OH2 WAT			11.659		1.00 43.46
40	7566	OH2 WAT			·	62.469 166.796	1.00 59.20
	7567	OH2 WAT					1.00 43.78
	7568	OH2 WAT				60.533 95.807	
	7569	OH2 WAT	M	279	40.776	65.445 180.203	1.00°55.54

	7570	OH2	WAT	W	280		-10.848	62.130	148.427	1.00	55.28
	7571			٠.	281		19.914	1, 1	134.430		
	7572				282		21.483		111.403	1.00	36.86
	7573	OH2	WAT	W	283		38.967		110.346		60.29
5	7574				284		1.572		152.361		37.17
	7575				285.		37.723		156.080		70.26
	7576				286		2.966	•	103.222		49.50
	7577				287		-1.589		102.705		73.77
	7578	OH2	WAT	· W	288		37.516	34.582			47.25
10	7579	OH2	WAT	W	289		18.845	•	161.444		58.39
	7580	OH2	WAT	. W	290		7.134		164.340		38.74
	7581	OH2	WAT	W	291		-5.751		111.073		38.80
	7582	ОН2	WAT	W	292	•	28.331	79,237	149.230		45.26
	7583	OH2	WAT	W	293		28.736	72.020	170.198	1.00	50.37
15	7584	OH2	WAT	M	294.		7.807	53.256	124.651	1.00	35.93
	7585	он2	WAT	W	295		5.276	73.692	117.621	1.00	48.57
	7586	OH2	WAT	W	296	,	25.199	57.397	157.092	1.00	56.90
	7587	ОН2	WAT	W	297		23.531	47.649	123.560	1.00	48.49
	7588	OH2	TAW	W	298		22.536	36.594	112.333	1.00	38.66
20	7589	OH2	WAT	W	299	,	21.236	80.762	157.102	1.00	43.11
	7590	OH2	WAT	W	300		43.516	82.149	164.770	1.00	51.55
	7591	OH2	WAT	W	301		24.994	36.436	113.441	1.00	33.28
	7592		WAT				35.020	50.272	154.159	1.00	45.25
							19.366	38.121	119.490	1.00	44.24
25	7594				304			43.321	164.662	1.00	52.52
	7595				305	·	28.803		185.096	1.00	62.39
	7596		WAT				20.912		136.612		50.93
	7597		WAT				-0.130		157.579		59.19
20	7598		TAW				-3.536		123.927		52.36
30	7599		TAW				1.063		115.474		37.76
	7600						38.405				
	7601				311				139.796		
	7602						17.857		169.577		
35	7603				313		32.002				
33							12.387				
					315		0.891				
	7606						41.633		127.755		47.27
•	7607		WAT				32.423				25.42
40							12.331		88.139		
1 0					319				144.764		
							40.548		157.210		43.00
	7611				321		22.089		98.234		
	7612	OHZ	WAT	٧V	222		7.239	64.978	154.179	1.00	37.09

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0.550 86.841 121.144 1.00 22.51
      7613 OH2 WAT W 323
                             24.184 50.980 99.752
      7614
           OH2 WAT W 324
                                                     1.00 47.16
      7615
           OH2 WAT W 325
                              23.665
                                     59.158 109.888
                                                    1.00 45.49
      7616
           OH2 WAT W 326
                                     52.728 98.891
                              19.813
                                                     1.00 46.97
  5
      7617
           OH2 WAT W 327
                              -2.839
                                     32.085 138.129
                                                    1.00 39.78
      7618
           OH2 WAT W 328
                               9.499
                                     62.749 103.240
                                                    1.00 46.62
      7619
           OH2 WAT W 329
                              7.415
                                     41.030 114.734
                                                     1.00 40.46
      7620
           OH2 WAT. W 330
                              -0.069
                                     86.118 130.467
                                                    1.00 49.80
           OH2 WAT W 331
                                     60.694 99.873 1.00 33.56
     7621
                              40.673
 10
     7622
           OH2 WAT, W 332
                                     50.697 121.483
                              14.416
                                                     1.00 64.77
     7623
           OH2 WAT W 333
                              24.011 78.487 155.905
                                                    1.00 38.04
     7624
           OH2 WAT W 334
                              20.533 77.071 160.985
                                                     1.00 58.11
     7625
           OH2 WAT W 335
                              23.195
                                     83.022 158.527
                                                     1.00 44.92
     7626 OH2 WAT W 336
                              16.270 78.813 129.819
                                                     1.00 54.00
 15
     7627
           OH2 WAT W 337
                              15.464 66.982 107.609 1.00 26.03
     7628
           OH2 WAT W 338
                                                     1.00 64.40
                             31.640 37.939 156.771
     7629 OH2 WAT W 339
                              46.976 64.163 165.205
                                                     1.00 36.91
     7630
           OH2 WAT W 340
                             33.304 48.195 153.946
                                                     1.00 52.87
     7631 OH2 WAT W 341
                             -1.048 39.586 149.790
                                                     1.00 44.96
20
     7632 OH2 WAT W 342
                             35.287 57.004 186.624
                                                     1.00 52.61
     7633
           OH2 WAT W 343
                             2.662 60.413 144.348
                                                     1.00 57.31
           OH2 WAT W 344
     7634
                             14.848 52.164 166.291
                                                     1.00 42.67
     7635 OH2 WAT W 345 4.916 39,701 110.853 1.00 50.26
     7636
           OH2 WAT W 346
                             26.538 38.184 115.313
                                                    1.00 30.74
25
     7637
           OH2 WAT W 347 34.541 89.227 153.452
                                                    1.00 50.57
     7638
           OH2 WAT W 348
                             16.788 48.259 160.825
                                                    1.00 33.71
     7639
           OH2 WAT W 349
                            35.250 49.549 156.822
                                                    1.00 55.52
     7640
           OH2 WAT W 350
                             -3.272 54.762 155.638
                                                    1.00 42.76
     7641
           OH2 WAT W 351
                             26.550 78.335 147.072
                                                    1.00 48.38
30
     7642
          OH2 WAT W 352
                             32.287 29.392 98.163
                                                    1.00 26.70
     7643
          OH2 WAT W 353
                             34.002
                                     66.690 112.543 1.00 45.32
     7644
           OH2 WAT W 354
                             0.508 65.282 103.717
                                                    1.00 52.50
     7645
          OH2 WAT W 355
                             4.524
                                     36.515 131.330
                                                    1.00 56.33
     7646
          OH2 WAT W 356
                             45.262
                                     59.545 161.086 1.00 41.72
35
     7647
          OH2 WAT W 357
                              4.961
                                     65.132 143.556 1.00 59.00
     7648
          OH2 WAT W 358
                             12.179
                                    86.053 112.142
                                                    1.00 38.89
     7649
          OH2 WAT W 359
                            32.530 38.766 141.377
                                                    1.00 47.21
     7650
          OH2 WAT W 360
                              6.570 81.549 111.394
                                                    1.00 44.16
     7651
          OH2 WAT W 361
                             13.004
                                    72.367 165.279 1.00 45.96
40
     7652
          OH2 WAT W 362
                                    68.206 100.661 1.00 67.06
                             31.973
    7653
          OH2 WAT W 363
                             44.263
                                    51.590 120.936 1.00 54.89
    7654
          OH2 WAT W 364
                                    47.302 147.740
                             30.071
                                                    1.00 47.85
    7655
          OH2 WAT W 365
                             20.166 55.086 98.322 1.00 37.15
```

	7656	OH2	WAT	W	366	15.595	43.155	106.386	1.00	66.70
	7657	OH2	WAT	W	367	-3.446	69.862	164.261	1.00	46.11
	7658	OH2	WAT	W	368	35.229	67.308	109.860	1.00	59.10
*	7659	OH2	WAT	W	369 [,]	20.753	88.034	127.140	1.00	46.69
5	7660	OH2	WAT	W	370	9.041	55.783	142.925	1.00	48.36
	7661	OH2	WAT	W	371	26.451	83.995	180.936	1.00	60.29
	7662	OH2	WAT	W	372	33.378	81.968	123.649	1.00	57.47
	7663	OH2	WAT	W	373	7.117	59.500	167.632	1.00	54.66
	7664	OH2	WAT	W	374	-13.134	61.653	154.371	1.00	37.87
10	7665	OH2	WAT	M	375	39.406	42.629	92.387	1.00	48.35
	7666	OH2	WAT	W	376	-1.509	54.871	151.229	1.00	50.25
	7667	OH2	WAT	M	377	2.526	67.268	166.696	1.00	68.89
	7668	OH2	WAT	M	378	42.944	66.027	151.239	1.00	61.53
	7669	OH2	WAT	W	379	-5.381	84.022	118.746	1.00	46.28
15	7670	OH2	WAT	W	380	25.886	36.345	89.108	1.00	44.82
	7671	OH2	WAT	W	381	36.757	88.320	174.167	1.00	46.84
	7672	OH2	WAT	W	382	9.522	77.097	151.130	1.00	49.50
	7673	OH2	WAT	W	383	27.175	43.869	121.483	1.00	64.70
	7674	OH2	WAT	W	384	25.188	89.834	168.031	1.00	29.17
20	7675	OH2	WAT	W	385	-2.133	41.763	107.962	1.00	55.32
	7676	ОН2	WAT	W	386	17.581	68.108	147.353	1.00	50.43
	7677	OH2	WAT	W	387	-2.716	54.084	153.333	1.00	47.42
	7678	OH2	WAT	W	388	1.214	58.353	145.206	1.00	54.87
	7679	OH2	TAW	W	389	32.478	44.660	97.842	1.00	36.41
25	7680	OH2	TAW	W	390	-0.526	39.840	108.033	1.00	60.43
	7681	OH2	WAT	W	391	49.539	60.328	164.723	1.00	48.42
	7682	OH2	WAT	M	392	-1.977	85.907	128.985	1.00	43.64
	7683	OH2	WAT	M	393	19.586	57.647	152.990	1.00	20.10
	7684		WAT			10.485	50.231	124.846	1.00	41.75
30	7685		WAT			44.275		80.377		
		OH2				-5.305	81.386	124.897		
	7687	OH2				8.432	55.753	124.650	1.00	41.19
	7688		WAT			13.851	49.974	119.218	1.00	31.25
٥.	7689		WAT			31.233		96.006	1.00	45.70
35	7690	OH2				19.392		89.688		52.10
	7691	OH2				21.499		106.290		56.95
	7692		WAT			38.194		107.570		38.44
	7693		TAW			19.114		85.421	1.00	37.30
	7694	OH2				40.014		88.531		44.55
40	7695	OH2					62.587			39.93
	7696		WAT				65.974			36.94
	7697					28.758			1.00	37.27
	7698	OH2	WAT	W	408	38.693	41.435	95.010	1.00	57.50

7699 OH2 WAT W 409 25.591 57.948 93.946 1.00 45.44 7700 OH2 WAT W 410 27.357 55.891 95.673 1.00 63.85

END

PCT/US02/38715

Table IB
Atomic Coordinates of UPPS in complex with FPP

							•									
	CR	YST1	58	8.i	08	44	.558	115	.535	90	.00	98.	69	90	0.00	
5	AT	OM	RE:	SID	UE		X		<u>y</u>	•	<u>Z</u>		<u>Oc</u>	<u>C</u>	<u>B</u>	
	1	СВ	GLU	A	14	,	-6.	102	26.5	64		502	1.	00	65.	83
	2	CG	GLU	Α	14		-7.	057	26.9	20	36.	373	1.	00	66.	40
	3	CD	GLU	A	.14		-6.	477	26.6	04	34.	993	1.	00	67.	15
	4	OE1	GLU	A	14		-7.	128	26.9	38	33.	975	1.	00	68.	21
10	5	OE2	GLU	Α	14	•	-5.	370	26.0	21	34.	921	1.	00	66.	67
	6	С	GLU	A	14		-4.	263 [.]	24.9	24	37.	894	1.	00	63.	83
	7	0	GLU	A	14		-3.	819	25.3	28	38:	969	1.	00	63.	93
	8	N	GLU	A	14		-6.	625	24.3	67	38.	522	1.	00	67.	24
	9	CA	GLU	A	14		-5.	741	25.0	79.	37.	555	1.	00	65.	39
15	10	N	VAI	A	. 15	•	-3	.500	24.	350	36	.966	1	.00	48	.09
	11	CA	VAI	A	15	•	-2	.072	24.	131	37	.182	. 1	.00	46	. 83
	12	СВ	VAL	A	15		-1	.842	23.	108	38	.340	1	.00	46	.56
	13	CG1	. VAL	A	15		-2	644	21.8	340·	38	.082	1	.00	51	.75
	14	CG2	VAL	A	15	٠	-0.	363	22.7	773	38	.479	. 1	.00	50	. 29
20	15	С	VAL	Α	15		-1.	.330	23.6	554	35	.931	1.	.00	43	.02
	16	0	VAL	Α	15		-1.	893	22.9	95	35	.044	1.	00	43.	. 85
	17	N	PRO	Α	16		-0.	048	24.0	004	35	.838	1.	00	43.	.32
	18	CD	PRO	Α	16	. 7.	0.	613	25.0	8,6	36,	582	, 1.	00	43.	32
	19	CA	PRO	A	16		0.	758	23.6	500	34.	690	1.	00	45.	94
25		CB	PRO	A	16		1.	936	24.5	73	34	734	1.	00	46.	50
	21	CG	PRO		16		1.	389	25.7	57	35.	498	1.	00	46.	71
	22	С	PRO	•	16		1.	212	22.1	.52	34.	830	1.	00	46.	22
	23	0	PRO		16		1.	215	21.5	90	35.	929	1.	00	44.	84
00	24	N	THR		17	,	1.	607	21.5	56	33.	713	1.	00	47.	29
30	25	CA	THR		17		2.	064	20.1	78	33.	727	1.	00	43.	32
	26	СВ	THR		17		1.	170	19.2	91	32.	879	. 1.	00	39.	41
	27	OG1	THR		17		-0.	198	19.5	11	33.	243	1.	00	43.	75
	28	CG2	THR		17			539	17.8	26	33.	084	1.	00	37.	92
25	29	C	THR		17			452	20.0		33.	149	1.	00	41.	03
35	30	0	THR		17			773	20.7		32.	162	1.	00	43.	88
	31	N	GLN		18			278	19.2		33.	760	1.	00	41.	44
	32	CA	GLN		18			614	19.0		33.	231	1.	00	41.	88
	33	CB	GLN		18				17.8		33.	993	1.	00	46.	62
40	34	CG	GLN		18			760	18.2		35.	417	1.	00	52.	25
40	35	CD	GLN		18			791	17.2	21	35.	947	1.0	00	57.	97
	36		GLN		18			915	17.1		35.	448	1.0	00	58.	34
	37		GLN					108	16.45		36.	958	1.0	00	52.	89
	38	С	GLN	A	18		5.3	345	18.5		31.	811	1.0	00	39.	78
									229	,						

	39	0	GLN	A	18		4.495	17.642	31.603	1.00	34.46
	40	N	VAL	A	19		6.041	19.089	30.836	1.00	41.79
	41	CA	VAL	Ą	19		5.838	18.682	29.452	1.00	43.01
	42	СВ	VAL	A	19	· -	5.263	19.845	28.599	1.00	43.44
5	43	CG1	VAL	Á	19		6.153	21.066	28,.705	1.00	47.93
	44	CG2	VAL	A	19		5.132	19.413	27.150	1.00	37.93
	45	С	VAL	A	19		7.143	18.184	28.837	1.00	41.23
	46	0	VAL	Α	. 19		8.130	18.915	28.775	1.00	42.44
	47	N	PRO	A	20		7.162	16.922	28.373	1.00	40.76
10	48	CD	PRO	A	20		5.990	16.042	28.223	1.00	38.76
	49	CA	PRO	A	20		8.344	16.306	27.760	1.00	38.00
	50	СВ	PRO	A	20		7.797	14.993	27.198	1.00	36.72
	51	CG	PRO	A	20		6.338	15.287	26.983	1.00	35.57
	52	С	PRO	A	20		9.015	17.164	26.694	1.00	35.22
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	65		HIS		22		15.045	12.798	21.009	1.00	27.15
	66	NE2	HIS		22		13.791	12.471	20.750	1.00	23.08
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30	68	0	HIS		22		11.089	13.415		1.00	24.16
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	70	CA	ILE		23		9.398	12.572	22.846		
	71	СВ	ILE		23		7.925	12.994	22.659		16.92
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35	73	CG1			23		7.495	13.927	23.797		16.92
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15	.225	CB	VAL	A	42	-1.361	-1.228	2.344	1.00	36.84
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	227	CG2	VAL	A	42	0.155	-1.107	2.221	1.00	31.91
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	237	CE2	PHE	A	43	-7.731	2.395	0.785	1.00	31.31
	238	CZ	PHE	A	43	-6.813	2.470	-0.258	1.00	29.07
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	242	CA	GLY	A	44	-3.512	2.362	7.763	1.00	43.50
	243	С	GLY	A	44	-2.251	3.185	7.894	1.00	40.10
	244	0	GLY	A	44	-2.189	4.130	8.681	1.00	40.32
35 ⁻	245	N	HIS	A	45	-1.242	2.823	7.114	1.00	33.52
	246	CA	HIS	A	45	0.015	3.539	7.133	1.00	30.60
	247	СВ	HIS	A	45	1.029	2.821	6.252	1.00	16.92
	248	CG	HIS	A	45	1.469	1.501	6.803	1.00	28.29
	249	CD2	HIS	A	45	2.701	0.954	6.934	1.00	34.82
40	250	ND1	HIS	A	45	0.582	0.560	7.277	1.00	34.82
	251	CE1	HIS	A	45	1.247	-0.511	7.675	1.00	39.36
	252	NE2	HIS	A	45	2.536	-0.297	7.477	1.00	40.10
	253	С	HIS	A	45	-0.169	4.986	6.686	1.00	34.04

	254	0	HIS	A	45		0.362	5.893	7.321	1.00	33.04
	255	N	LYS	S A	46		-0.918	5.226	5.613	1.00	37.67
	256	CA	LYS	S A	46		-1.112	6.606	5.190	1.00	36.56
	257	СВ	LYS	S A	46		-2.029	6.714	3.981	1.00	27.77
5	258	CG	LYS	A	46		-2.167	8.154	3.490	1.00	36.67
	259	CD	LYS	A	46		-2.906	8.248	2.160	1.00	47.11
	260	CE	LYS	a A	46	,	-2.187	7.465	1.060	1.00	45.30
	261	NZ	LYS	A	46		-2.935	7.463	-0.231	1.00	54.67
	262	С	LYS	A	46		-1.737	7.348	6.350	1.00	35.24
10	263	0	LYS	A	46		-1.280	8.429	6.723	1.00	34.48
	264	N	ALA	À	47		-2.781	6.757	6.924	1.00	34.22
	265	CA	ALA	A	47		-3.462	7.358	8.069	1.00	33.65
	266	СВ	ALA	A	47		-4.588	6.451	8.550	1.00	22.25
	267	С	ALA	A	47		-2.457	7.601	9.201	1.00	33.26
15	268	0	ALA	A	47		-2.505	8.632	9.876	1.00	35.94
	269	N	GLY	Α	48		-1.558	6.643	9.413	1.00	31.73
	270	CA	GLY	Α	48		-0.562	6.814	10.443	1.00	31.22
	271	С	GLY	Α	48		0.056	8.162	10.156	1.00	28.17
	272	0	GLY	Α	48		0.063	9.050	11.005	1.00	30.21
20	273	N	MET	A	49		0.546	8.321	8.933	1.00	26.41
	274	CA	MET	A	49	,	1.168	9.565	8.510	1.00	26.13
	275	CB	MET	Α	49		1.525	9.501	7.019	1.00	26.11
	276	CG	MET	A,	49		1.999	10.831	6.415	1.00	31.14
	277	SD	MET	A	49		2.596	10.723	4.688	1.00	30.86
25	278	CE	MET		49		1.149	10.009	3.871	1.00	27.72
	279	С	MET	A	49		0.267	10.764	8.780	1.00	26.86
	280	0	MET	A	49		0.740	11.812	9.209	1.00	25.74
-	281	N	GLU	A	50		-1.028	10.621	8.532	1.00	26.86
•	282	CA	GLU		50		-1.943	11.725	8.780	1.00	29.13
30	283	CB	GLU,	A	50		-3.364	11.333	8.397	1.00	35.38
	284	CG	GLU		50		-3.465	10.916	6.948	1.00	42.20
	285	CD	GLU		50		-4.615			1.00	55.85
	286		GLU		50		-4.707			1.00	54.70
25	287		GLU		50		-5.414			1.00	62.59
35	288	C	GLU		50		-1.885	•			33.72
	289	0	GLU		50		-1.701	13.311	10.566		40.50
	290	N	ALA		51		-2.031		11.143		30.97
	291	CA	ALA		51		-1.972		12.560		29.01
40	292	CB	ALA		51		-2.288		13.384		33.60
40	293	C	ALA		51		-0.587	12.009	12.910		28.16
	294	0	ALA		51		-0.448		13.835		28.15
	295	N	LEU		52		0.439		12.182		26.73
	296	CA	LEU	A	52		1.785	12.051	12.475	1.00	26.65

	297	СВ	LEU	Α	52		2.809	11.478	11.499	1.00	16.92
	298	ÇG	LEU	A	52		4.267	11.370	11.979	1.00	16.92
	299	CD1	LEU	A	52		5.184	11.281	10.768	, 1.00	16.92
	300	CD2	LEU	Å	52	*	4.661	12.570	12.823	1.00	22.52
5	301	С	LEU	·A	5,2		1.765	13.561	12.338	1.00	32.69
	302	0	LEU	A	52	• •	2.309	14.273	13.180	1.00	34.28
	303	N	GLN	A	53		1.124	14.041	11.272	1.00	32.34
	304	ĆA	GLN	Α	53		1.016	15.475	11.005	1.00	28.24
	305	СВ	GLN	A	53		0.241	15.729	9.714	1.00	22.43
10	306	CG	GLN	Ą	53		0.219	17.194	9.297	1.00	16.92
	307	CD	GLN	A	53		1.467	17.602	8.535	1.00	16.92
	308	OE1	GLN	A	53		2.512	16.956	8.631	1.00	26.60
	309	NE2	GLN	A	53		1.364	18.685	7.779	1.00	16.92
	310	С	GLN	A	53		0.302	16.180	12.150	1.00	31.47
15	311	0	GLN.	Α	53	·	0.740	17.227	12.618	.1.00	30.88
	312	N	THR	A	54	•	-0.809	15.598	12.583	1.00	32.71
	313	CA	THR	A.	54		-1.599	16.137	13.679	1.00	29.40
	314	CB	THR	A	54		-2.824	15.282	13.932	1.00	22.85
	315	OG1	THR	A	54		-3.692	15.346	12.796	1.00	33.45
20	316	CG2	THR	A	54		-3.545	15.751	15.186	1.00	16.92
	317	С	THR	A	54		-0.819	16.176	14.977	1.00	32.23
	318	0	THR	A	54		-0.781	17.197	15.652	1.00	35.38
	319	Ņ	VΑĻ	Α	55,		-0.219	15.049	15.337	1.00	33.35
	320	CA	VAL	A	55		0.552	14.958	16.568	1.00	32.18
25	321	CB	VAL	A	55		1.029	13.501	16.835	1.00	26.17
	322		VAL		55		1.962	13.460	18.026	1.00	16.92
	323	CG2	VAL	A	55		-0.164	12.606	17.105	1.00	28.32
	324	С	VAL		55		1.760	15.875	16.514	1.00	32.33
	325	0	VAL		55		1.981	16.666	17.429	1.00	31.60
30	326	N	THR		56		2.531	15.773	15.435	1.00	31.81
	327	CA	THR		56		3.732	16.582	15.266	1.00	36.75
	328	СВ	THR		56		4.422	16.248	13.924	1.00	33.23
	329	OG1	THR	A	56		5.715	16.861	13.877	1.00	35.26
0.5	330	CG2	THR		56		3.599	16.758	12.764	1.00	48.73
35	331	С	THR		56		3.416	18.082	15.341	1.00	40.46
	332	0	THR		56		4.227	18.881	15.801	1.00	43.12
	333	N	LYS		57		2.222	18.450	14.897	1.00	42.26
	334	CA	LYS		57		1.774	19.838	14.907	1.00	43.45
	335	CB	LYS	A	57		0.629	19.988	13.907	1.00	47.22
40	336	CG	LYS		57		0.464	21.352	13.292		47.96
	337	CD	LYS		57		-0.497	21.262	12.116		49.91
	338	CE	ĻYS		57		-1.823	20.642	12.534		55.23
	339	NZ.	LYS	A	57		-2.759	20.430	11.394	1.00	63.19
		•									

	240	•	T V/O	70	- 7	1 201.	20 167	16.324	1.00 4	4 75
	340 341	C	LYS		57 57	1.301 1.783	20.167	16.955	1.00 4	
		N	ALA		58	0.359	19.377	16.819	1.00 4	
	342		ALA		58	-0.174	19.557	18.158	1.00 4	
5	343	CA			58		18.379	18.520	1.00 3	
ی	344	CB	ALA			-1.048		19.165	1.00 4	_
	345	C	ALA		58	0.957	19.682		1.00 4	
	346	0	ALA		58	0.940	20.550	20.028	1.00 4	
	347	N	ALA	*	59	1.941	18.800	19.046	1.00 4	
10	348	CA	ALA		59	3.085	18.785	19.948	1.00 4	
10	349	CB	ALA		59	3.934		19.682		
	350	C	ALA		59	3.931	20.035	19.802	1.00 4	
	351	0	ALA		59	4.663	20.409	20.714	1.00 4	
	352	N	ASN		60	3.830	20.680	18.646	1.00 5	
1.5	353	CA	ASN		60	4.599	21.891	18.380	1.00 5	
15	354	CB	ASN		60	4.661	22.151	16.870	1.00 5	,
	355	CG	ASN		60	5.519	23.346	16.516	1.00 5	
	356		ASN		60	6.699	23.405	16.855	1.00 5	
	357		ASN		60	4.927	24.306	15.820	1.00 6	
20	358	C,	ASN		60	3.998	23.099	19.095	1.00 4	
20	359	0	ASN		60	4.729	23.925	19.648	1.00 4	
	360	N	LYS		61	2.668	23.189	19.091	1.00 4	
	361	CA	LYS		61	1.978	24.296	19.739	1.00 4	
	362	CB	LYS		61	0.494	24.296	19.378	1.00 3	
	363	CG	LYS		61	-0.376	23.520	20.360	1.00 4	
25	364	CD	LYS		61	-1.847	23.893	20.228	1.00 6	
	365	CE	LYS	A	61	-2.674	23.282	21.355	1.00 7	6.26
	366	NZ	LYS.		61	-4.111	23.687	21.306		7.30
	367	С	LYS		61	2.105	24.171	21.247	1.00 4	
•	368	0	LYS		61	1.872	25.120	21.987	1.00 3	
30	369	N	LEU		62	2.470	22.982	21.697	1.00 4	
	370	CA	LEU		62	2.598	22.724	23.117	1.00 4	
	371	CB	LEU		62	2.047	21.331	23.436	1.00 4	
	372	CG	LEU		62	1.512	21.076	24.843	1.00 4	
	373		LEU		62	0.465	22.122	25.216	1.00 4	
35	374	CD2	LEU		62	0.909	19.691	24.888	1.00 4	1.95
	375	С	LEU	Α	62	4.043	22.852	23.572	1.00 3	7.78
	376	0	LEU	A	62	4.361	22.576	24.721	1.00 3	6.77
	377	N	GLY	A	63	4.919	23.254	22.662	1.00 3	4.00
•	378	CA	GLY	A	63	6.310	23.445	23.026	1.00 3	4.47
40	379	С	GLY	A	63	7.250	22.257	23.130	1.00 3	4.70
	380	0	GLY	A	63	8.370	22.399	23.623	1.00 3	7.15
	381	N	VAL	A	64	6.830	21.078	22.703	1.00 3	2.50
	382	CA	VAL	A	64	7.745	19.951	22.764	1.00 3	3.85

	383	СВ	IAV	A	64	7.075	18.672	22.254	1.00	38.31
	384	CG:	1 VAI	A	64	8.104	17.563	22.102	1.00	45.70
	385	CG2	2 VAI	A	64	5.981	18.254	23.216	1.00	30.49
	386	С	· VAI	A	64	8.923	20.305	21.861	1.00	32.11
5	387	0	VAI	A	64	8.738	20.626	20.693	1.00	35.71
	388	N	LYS	A	65	10.133	20.264	22.398	1.00	30.11
,	389	CA	LYS	A	65	11.301	20.604	21.598	1.00	32.19
	390	СВ	LYS	A S	65	12.555	20.633	22.464	1.00	34.45
	391	CG	LYS	A	65	13.133	22.024	22.668	1.00	28.19
- 10	392	CD	LYS	A	65	12.183	22.927	23.451	1.00	32.70
	393	CE	LYS	A	65	12.850	24.251	23.841	1.00	50.92
	394	NZ	LYS	A	65	14.038	24.082	24.743	1.00	60.18
	395	С	LYS	A	65	11.542	19.683	20.411	1.00	32.24
	396	0	LYS	Α	65	11.799	20.154	19.307	1.00	32.31
15	397	N	VAL	A	66	11.466	18.374	20.634	1.00	29.19
	398	CA	VAL	A	66	11.695	17.399	19.561	1.00	27.66
	399	СВ	VAL	A	66	13.232	17.130	19.391	1.00	30.38
	400	CG1	. VAL	A	66	13.926	17.314	20.720	1.00	29.01
	401	CG2	VAL	Α	66	13.498	15.717	18.840	1.00	16.92
20	402	С	VAL	A	66	10.970	16.069	19.763	1.00	22.57
	403	0	VAL	A	66	10.605	15.725	20.879	1.00	18.50
	404	N	ILE	A	67	10.730	15.346	18.670	1.00	23.89
,	405	CA	ILE	A	67	10.099	14.028	18.744	1.00	3124
	406	CB	ILE	A	67	8.541	14.075	18.622	1.00	30.49
25	407	CG2	ILE	A	67	7.963	14.971	19.709	1.00	32.00
	408	CG1	ILE	A	67	8.113	14.561	17.242	1.00	35.49
	409	CD1	ILE	A	67	6.610	14.613	17.079	1.00	44.48
	410	С	ILE	A	67	10.671	13.104	17.674	1.00	32.32
	411	0	ILE	A	67	10.849	13.495	16.512	1.00	36.35
30	412	N	THR	A	68	10.988	11.885	18.100	1.00	27.06
	413	CA	THR	A	68	11.554	10.866	17.229	1.00	22.58
	414	CB	THR	A	68	12.836	10.287	17.823	1.00	20.26
	415	OG1	THR	A	68	13.811	11.331	17.956	1.00	31.06
	416	CG2	THR	A	68	13.373	9.182	16.937	1.00	16.92
35	417	С	THR	A	68	10.540	9.750	17.040	1.00	26.08
	418	0	THR	A	68	10.226	9.008	17.969	1.00	28.24
	419	N	VAL	A	69	10.028	9.657	15.818	1.00	25.72
	420	CA	VAL	A	69	9.022	8.677	15.450	1.00	22.44
	421	CB	VAL	A	69	8.025	9.297	14.488	1.00	20.89
40	422	CG1	VAL	A	69	7.234	10.378	15.180	1.00	16.92
	423	CG2	VAL	A	69	8.770	9.892	13.313	1.00	16.92
	424	С	VAL	A	69	9.667	7.490	14.770	1.00	23.00
	425	0	VAL	A	69	10.401	7.652	13.794	1.00	23.85

	426	N	TYR	Α	70	9.399	6.299	15.295	1.00	25.89
	427	CA	TYR	A	70	9.943	5.066	14.727	1.00	26.71
	428	CB	TYR	A	70	9.802	3.916	15.728	1.00	22.08
	429	CG	TYR	A.	70.	10.817	2.805	15.552	1.00	16.92
5	430	CD1	TYR	Α	70	11.756	2.842	14.518	1.00	16.92
	431	CE1	TYR	Α	70	12.708	1.834	14.374	1.00	16.92
	432	CD2	TYR	A	70	10.856	1.723	16.440	1.00	18.76
	433	CE2	TYR	A	70	11.802	0.710	16.306	1.00	20.19
	434	CZ	TYR	À	70 .	12.723	0.774	15.272	1.00	23.85
10	435	ОН	TYR	A	70	13.660	-0.218	15.136	1.00	28.88
	436	С	TYR	Α	70	9.150	4.752	13.454	1.00	27.42
	437	0	TYR	Α	70 .	8.125	4.053	1,3.508	1.00	29.24
•	438	N	ALA	A	71	9.640	5.272	12.324	1.00	26.20
	439	CA	ALA	A	71	9.004	5.115	11.013	1.00	27.77
15	440	СВ	ALA	Α	71 ·	9.336	6.326	10.149	1.00	21.40
	441	С	ALA	Α	71	9.302	3.821	10.232	1.00	33.28
	442	0	ALA	Α	71	8.441	3.314	9.513	1.00	35.06
	443	N	PHE	A	72	10.514	3.292	10.344	1.00	34.13
	444	CA	PHE	A	72	10.837	2.055	9.640	1.00	35.25
20	445	СВ	PHE	A	72	11.105	2.336	8.152	1.00	28.54
	446	CG	PHE	Α	72	11.098	1.096	7.289	1.00	32.61
	447	CD1	PHE	Α	72	9.897	0.518	6.880	1.00	33.56
	448	CD2	PHE	Α,	72	12.290	0.478	6.917	1.00	35.80
	449	CE1	PHE	Α	72 " " "	9.885	-0.661	6.113	1.00	28.42
25	450	CE2	PHE	A	7.2	12.283	-0.698	6.154	1.00	32.48
	451	CZ	PHE	A	72	11.077	-1.265	5.753	1.00	31.11
	452	С	PHE	A	72	12.053	1.386	10.275	1.00	40.63
	453	0	PHE	A	72	13.172	1.865	10.135	1.00	43.32
•	454	N	SER	A	73	11.832	0.280	10.980	1.00	47.02
30	455	CA	SER	A	73	12.932	-0.435	11.627	1.00	49.68
	456	CB	SER	A	73	12.409	-1.381	12.708	1.00	43.74
	457	OG	SER	A	73	12.032	-2.624	12.145	1.00	33.26
	458	С	SER	A	73	13.703	-1.250	10.601	1.00	52.36
	459	0	SER	A	73	13.227	-1.477	9.487	1.00	53.00
35	460	N	THR	A	74	14.893	-1.697	10.985	1.00	57.20
	461	CA	THR	A	74	15.726	-2.488	10.092	1.00	62.04
	462	CB	THR	A	74	17.131	-2.742	10.714	1.00	67.14
	463	OG1	THR	A	74	17.593	-1.557	11.374	1.00	74.37
	464	CG2	THR	A	74	18.136	-3.103	9.632	1.00	71.77
40	465	С	THR	A	74	15.027	-3.826	9.856	1.00	62.95
	466	O .	THR	A	74	15.157	-4.441	8.798	1.00	62.39
	467	N	GLU	A	75	14.256	-4.252	10.850	1.00	63.63
	468	CA	GLU	A	75	13.553	-5.525	10.786	1.00	66.15

	469	СВ	GLU	Α	75	13.387	-6.084	12.203	1.00 75.90
	470	CG	GLU	A	75 ·	12.911	-7.521	12.255	1.00 93.53
	471	CD	GLU	A	75	12.685	-8.000	13.669	1.00103.81
	472	OE1	GLU	Α	75	11.907	-7.347	14.399	1.00110.70
5	473	OE2	GLU	A	75	13.283	-9.030	14.048	1.00111.36
	474	C	GLU	A	75	12.193	-5.457	10.096	1.00 66.40
	475	0	GLU	A	75	11.395	-6.390	10.193	1.00 68.91
	476	N	ASN	A	76	11.925	-4.362	9.393	1.00 64.57
	477	CA	ASN	A.	76	10.646	-4.222	8.702	1.00 59.63
10	478	СВ	ASN	A	76	10.136	-2.778	8.788	1.00 53.70
	479	CG	ASN	A	76	9.370	-2.506	10.066	1.00 46.89
	480	OD1	ASN	A	76	8.523	-3.299	10.470	1.00 50.66
	481	ND2	ASN	A	76 .	9.652	-1.377	10.700	1.00 40.20
	482	С	ASN	A	76	10.685	-4.656	7.240	1.00 56.27
15	483	0	ASN	A	76	9.636	-4.897	6.642	1.00 55.41
	484	N	TRP	A	77	11.882	-4.763	6.666	1.00 53.67
	485	CA	TRP	A	77	12.007	-5.160	5.266	1.00 51.94
	486	CB	TRP	A	77	13.469	-5.096	4.805	1.00 48.90
	487	CG	TRP		77	14.125	-3.744	4.934	1.00 51.60
20	488	CD2	TRP	A	77	14.156	-2.698	3.948	1.00 51.70
	489	CE2	TRP		77	14.900	-1.627	4.497	1.00 52.11
	490	CE3	TRP		77	13.628	-2.561	2.655	1.00 43.86
	491	CD1	TRP		77	14.826	-3.274	6.007	1.00 52.12
0.5	492	NE1	TRP		77	15.295		5.752	1.00 53.74
25·	493	CZ2			77	15.130	-0.436	3.799	1.00 43.91
	494	CZ3	TRP		77	13.859	-1.369	1.960	1.00 37.41
	495	CH2	TRP		77	14.605	-0.326	2.537	1.00 35.61
	496	С	TRP		77	11.466	-6.574	5.063	
20	497	0	TRP		77	11.212	-7.006	3.935	1.00 54.30
30	498	N	THR		78	11.286	-7.280	6.172	1.00 46.30
	499	CA	THR		78	10.778		6.171	1.00 40.87
	500	CB	THR		78	10.756		7.602	1.00 40.94
	501	OG1			78	12.097	-9.255	8.103	1.00 41.23
35	502	CG2			78 70		-10.585	7.642	1.00 43.72
<i>J J</i>	503	C	THR		78 78	9.370	-8.747	5.597	1.00 39.63
	504	0	THR			8.927	-9.828	5.208	1.00 43.77
	505	N CD	ARG		79 70	8.671	-7.616	5.540	1.00.33.93
	506	CA	ARG		79 70	7.294		5.044	1.00 29.09
40	507	CB	ARG		79 70	6.661	-6.236	5.455	1.00 22.71
40	508	CG	ARG		79		-6.105		1.00 24.31
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	557	CA	LYS	A	85		6.804	-0.646	-1.669	.1.00	35.59
	558	СВ	LYS	Α	85		6.140	-1.478	-2.783	1.00	48.55
5	559	CG	LYS	Ά	85		5.367	-0.707	-3.855	1.00	59.03
	560	CD	LYS	A	85		6.264	-0.085	-4.912	1.00	67.33
	561	CE	LYS	A	85		5.426	0.664	-5.948	1.00	72.93
	562	NZ	LYS	Α	85		6.266	1.391	-6.950	1.00	68.29
	563	С	LYS	A	85		5.956	0.576	-1.290	1.00	33.73
10	564	0	LYS	Α	85 ·		6.393	1.716	-1.434	1.00	32.87
	565	N	PHE	A	86		4.760	0.305	-0.771	1.00	34.91
	566	CA	PHE	A	86	•	3.796	1.318	-0.334	1.00	38.00
	567	СВ	PHE	A	86		2.579	0.617	0.286	1.00	29.90
	568	CG	PHE	A	86		1.520	1.553	0.814	1.00	28.19
15	569	CD1	PHE	·Α	86		0.306	1.694	0.150	1.00	28.34
	570	CD2	PHE	A	86	•	1.703	2.237	2.014	1.00	30.14
	571	CE1	PHE	A	86		-0.714	2.495	0.678	1.00	16.92
	572	CE2	PHE	A	86		0.692	3.039	2.547	1.00	31.79
	573	CZ	PHE	Α	86		-0.519	3.166	1.879	1.00	23.42
20	574	С	PHE	A	86		4.372	2.317	0.671	1.00	41.33
	575	0	PHE	A	86, ·		4.384	3.522	0.413	1.00	44.39
	576	N	ILE	A	87		4.828	1.817	1.820	1.00	42.94
	577	CA	ILĘ	Α	87		,5, 390,	2.670	2.870	, 1.,00	44.91
	578	СВ	ILE	A	87		5.999	1.842	4.021	1.00	33.27
25	579	CG2	ILE	A	87		6.499	2.760	5.114	1.00	35.47
	580	CG1	ITE	Α	87		4.951	0.912	4.614	1.00	33.55
	581	CD1	ILE	A	87		5.500	0.015	5.692	1.00	34.35
	582	С	ILE		87		6.485	3.585	2.341	1.00	49.45
	583	0	ILE		87		6.391	4.805	2.460	1.00	51.81
30	584	N	MET	Α	88		7.519	2.990	1.756	1.00	49.47
	585	CA	MET	A	88		8.635	3.762	1.226	1.00	49.30
	586	СВ	MET		88		9.641	2.842	0.525	1.00	50.22
	587	CG	MET		88		10.269	1.771	1.418	1.00	45.64
a =	588	SD	MET		88		11.035	2.374	2.938	1.00	36.68
35	589	CE	MET		88		12.225	3.505	2.300	1.00	32.68
	590	С	MET		88		8.226	4.897	0.281	1.00	47.36
	591	0	MET		88		9.031	5.777	-0.022	1.00	47.71
	592	N	ASN		89		6.988	4.898	-0.194	1.00	47.87
	593	CA	ASN	A	89		6.582	5.981	-1.074	1.00	53.55
40	594		ASN		89		5.710	5.476	-2.219	1.00	59.69
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	597	ND2	ASN .	A	89		4.249	6.994	-3.411	1.00	59.82

	598	С	ASN	A	89		5.828	7.053	-0.300	1.00 54.69
	599	0	ASN	A	89		5.351	8.034	-0.875	1.00 55.77
	600	N	LEU	A	90		5.718	6.851	1.010	1.00 53.91
	601	CA	LEU	A	90		5.039	7.803	1.877	1.00 50.26
5	602	СВ	LEU	A	90		4.694	7.152	3.218	1.00 44.32
	603	CG	LEU	A	90		3.552	6.134	3.213	1.00 38.54
	604	CD1	LEU	A	90		3.422	5.504	4.582	1.00 43.04
	605	CD2	LEU	A	90		2.258	6.821	2.830	1.00 42.59
	606	С	LEU	A	90		5.909	9.039	2.091	1.00 47.14
10	607	0	LEU	A	90		5.391	10.136	2.305	1.00 44.55
	608	N	PRO	A	91		7.247	8.875	2.061	1.00 46.27
	609	CD	PRO	A	91		7.996	7.616	2.220	1.00 44.80
	610	CA	PRO	A	91		8.140	10.024	2.247	1.00 46.47
	611	СВ	PRO	A	91		9.521	9.376	2.300	1.00 43.34
15	612	CG	PRO	A	91		9.234	8.073	2.951	1.00 45.54
	613	С	PRO	Α	91		8.009	11.030	1.094	1.00 47.41
	614	0	PRO	A	91		8.412	12.186	1.208	1.00 46.38
	615	N	VAL	A	92		7.442	10.578	-0.020	1.00 47.94
	616	CA	VAL	A	92		7.249	11.439	-1.180	1.00 45.52
20	617	CB	VAL	A	92		7.204	10.622	-2.467	1.00 34.17
	618	CG1	VAL	A	92		7.081	11.547	-3.642	1.00 38.02
	619	CG2	VAL	A	92		8.456	9.775	-2.583	1.00 38.64
	620	С	VAL	A	92		5.940	12.205	-1.026	1.00 45.50
1	621	0	VAL	A	92		5.919	13.431	-1.117	1.00 44.68
25	622	N	GLU	A	93		4.851	11.476	-0.791	1.00 42.90
	623	CA	GLU	A	93		3.557	12.103	-0.582	1.00 42.53
	624	CB	GLU	A	93		2.522	11.082	-0.124	1.00 49.87
	625	CG	GLU	A	93		2.449	9.818	-0.951	1.00 57.60
	626	CD	GLU	A	93		1.189	9.021	-0.657	1.00 61.78
30	627	OE1	GLU	A	93		1.046	7.896	-1.187	1.00 71.50
	628	OE2	GLU	A	93		0.337	9.531	0.105	1.00 52.19
	629	С	GLU	A	93		3.753	13.110	0.539	1.00 43.12
	630	0	GLU	A	93		3.322	14.255	0.452	1.00 45.85
	631	N	PHE	A	94		4.414	12.664	1.601	1.00 45.41
35	632	CA	PHE	A	94		4.678	13.514	2.752	1.00 46.26
	633	CB	PHE	A	94		5.575	12.787	3.756	1.00 42.53
	634	CG	PHE	A	94		5.711	13.507	5.067	1.00 32.85
	635	CD1	PHE	A	94		4.633	13.568	5.956	1.00 28.47
•	636	CD2	PHE	A	94	•	6.894	14.167	5.396	1.00 28.12
40	637	CE1	PHE	A	94		4.726	14.279	7.153	1.00 19.92
	638	CE2	PHE	A	94	,	6.999	14.882	6.590	1.00 31.07
	639	CZ	PHE	A	94		5.909	14.936	7.468	1.00 25.79
	640	С	PHE	A	94		5.346	14.817	2.326	1.00 45.67

	641	_	DUE	71	0.4	4.858	15.901	2.636	1.00 41.22
	641 642	O N	PHE TYR		94 95	6.462	14.706	1.613	1.00 44.67
	643	CA	TYR		95	7.185	15.884	1.154	1.00 42.71
	644	CB	TYR		95	8.467	15.487	0.430	1.00 44.48
5	645	CG	TYR		95	9.245	16.675	-0.099	1.00 45.34
J	646	CD1			95	9.725	17.655	0.764	1.00 46.34
	647		TYR		95	10.449	18.740	0.292	1.00 50.00
	648		TYR		95	9.509	16.814	-1.458	1.00 46.57
	649		TYR		95	10.230	17.895	-1.938	
10	650	CEZ	TYR		95	10.700	18.853	-1.058	1.00 53.17
10	651		TYR		95	11.434	19.918	-1.521	1.00 55.77
	652	C	TYR		95	6.352	16.738	0.215	1.00 41.47
	653	0	TYR		95	6.237	17.951		1.00 41.47
	654	N	ASP		96	5.782	16.105	-0.804	1.00 38.09
15	655	CA	ASP		96	4.975	16.838	-1.761	1.00 34.86
15	656	СВ	ASP		96	4.278	15.907	-2.751	1.00 28.63
	657	CG	ASP		96	5.178	15.499	-3.898	1.00 32.06
	658		ASP		96	6.190	16.203	-4.142	1.00 29.64
	659		ASP		96	4.857	14.482	-4.561	1.00 33.25
20	660	С	ASP		96	3.924	17.694	-1.100	1.00 31.39
	661	0	ASP		96	3.933	18.908	-1.268	1.00 31.77
	662	N	ASN		97	3.025	17.087	-0.335	1.00 26.14
	663	CA	ASN		97	1.976	17.889	0.269	1.00 29.32
•	664	СВ	ASN		97	0.650	17.565	-0.433	1.00 34.58
25	665	CG	ASN		97	0.375	16.077	-0.515	1.00 33.64
	666		ASN		97	-0.464	15.628	-1.310	1.00 31.70
	667		ASN		97	1.067	15.299	0.319	1.00 25.32
	· 668	С	ASN		97	1.790	17.924	1.791	1.00 33.75
	669	0	ASN		97	0.826	18.521	2.275	1.00 31.16
30	670	N	TYR		98	2.699	17.319	2.552	1.00 37.18
	671	CA	TYR	A	98	2.586	17.361	4.012	1.00 35.12
	672	СВ	TYR	A	98	2.683	15.966	4.605	1.00 33.51
	673	CG	TYR	A	98	1.360	15.282	4.649	1.00 29.03
	674	CD1	TYR	A	98.	0.990	14.378	3.656	1.00 24.71
35	675	CE1	TYR	A	98	-0.266	13.797	3.651	1.00 19.15
	676	CD2	TYR	A	98	0.445	15.589	5.645	1.00 24.62
	67 7	CE2	TYR	A	98	-0.814	15.022	5.655	1.00 22.79
	678.	CZ	TYR	A	98	-1.168	14.125	4.652	1.00 25.75
	679	ОН	TYR	A	98	-2.433	13.574	4.644	1.00 31.99
40	680	С	TYR	A	98	3.645		4.649	1.00 36.88
	681	0	TYR	A	98	3.412	18.883	5.691	1.00 38.14
	682	N	VAL	A	99	4.811	18.293	4.012	1.00 34.30
	683	CA	VAL	A	99	5.932	19.105	4.465	1.00 27.39

	601	CP.	VAL	7\	99		7.193	18.760	3.658	1.00	20.34
•	684 685	CB CG1	VAL		99		8.284	19.772			16.92
	686		VAL		99		7.661		4.021	1.00	19.75
	687	С	VAL		99		5.646	20.614		1.00	31.44
5	688	0	VAL				6.009	21.371			35.10
_	689	N			100		4.991	21.072		1.00	34.59
	690	CD			100		4.444	20.363		1.00	35.82
	691	CA			100		4.706	22.502		1.00	33.54
	692	CB			100		3.679	22.561	2.064		31.42
10	693	CG			100		4.144	21.503	1.162	1.00	35.80
	694	С			100		4.147	23.037	4.490		34.59
	695	0	PRO	A	100		4.646	24.024	5.027	1.00	36.94
	696	N	GLU	A	101	,	3.117		5.002	1.00	33.67
	697	CA	GLU	A	101		2.481	22.785	6.245	1.00	,31.97
15	698	СВ	GLU	A	101		1.248	21.937	6.533	1.00	16.92
	699	CG	GLU	A	101		0.725	22.160	7.935	1.00	16.92
	700	ÇD	GĽŮ	A	101		-0.679	21.648	8.139	1.00	26.55
•	701	OE1	GLU	Α	101		-0.967	20.504	7.711	1,00	21.07
	702	OE2	GLU	A	101		-1.484	22.396	8.743	1.00	22.12
20	703	С	GLU	A	101	•	3.394	22.744	7.459	1.00	33.18
	704	0	GLU	A	101		3.421	23.682	8.258	1.00	32.52
	705	N	LEU	A	102		4.121	21.648	7.624	1.00	33.81
	706	CA	LEU	A,	102		5.019	21.560	8.756	1.00	31,47
	707	CB	LEU	À	102	<i></i>	5.820	20.262	8.694	1.00	30.43
25	708	CG	LEU	A	102		4.974	18.997	8.837	1.00	34.74
	709	CD1	LEU	Α	102		5.866	17.776	8.764	1.00	25.10
	710	CD2	LEU	A	102		4.232	19.029	10.162	1.00	36.87
	711	С	LEU	Α	102		5.942	22.769		1.00	30.29
	712	0	LEU				6.206		9.694	1.00	33.60
30	713	N			103		6.398	23.067	7.471		28.12
	714	CA			103		7.298		7.214		30.58
	715	СВ			103		7.735				32.00
	716	CG	HIS				8.864	25.083	5.451		35.36
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35	718		HIS				10.104		6.042		38.53
	719		HIS				10.909	25.894			36.15
	720		HIS				10.235	26.608			34.36
	721	C	HIS				6.677	25.552			31.60
40	722	0	HIS				7.365	26.488	7.931		26.65
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	727	0		A 104	4.762		9.631		40.90
	728	N		A 105	4.580		9.773		32.79
	729	CA		A 105	4.543	25.899	11.233		29.90
	730	CB		A 105	3.645	24.762			42.45
5	.731	CG	ASN	A 105	2.169	25.048	11.509		48.96
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	735	0	ASN .	A 105	6.030	25.474	13.075	1.00	24.21
10	736	N	ASN .	A 106	6.950	26.228	11.167	1,00	21.42
	737	CA	ASN .	A 106	8.314	26.278	11.687	1.00	21.95
	738	CB	ASN .	A 106	8.390	27.294	12.834	1.00	16.92
	739	CG	ASN .	A 106	9.818	27.682	13.180	1.00	18.90
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	742	С	ASN Z	A 106	8.854	24.937	12.177	1.00	26.82
	743	0	ASN A	A 106	9.655	24.892	13.111	1.00	28.64
	744	N	VAL 2	A 107	8.430	23.842	11.561	1:00	28.06
	745	CA	VAL Z	A 107	8.914	22.538	11.988	1.00	25.22
20	746	CB	VAL A	A 107	7.825	21.456	11.791	1.00	24.13
	747	CG1	VAL Z	A 107	8.322	20.100	12.286	1.00	37.12
	748	CG2	VAL Z	A 107	6.560	21.865	12.528	1.00	24.46
	749	Ċ	VAĻ 1	A 107	10.152	22.172	11.176	1.00	28.07
	750	0	VAL A	A 107	10.168	22.351	9.962	1.00	33.25
25	751	N	LYS A	A 108 ·	. 11.199	21.698	11.847	1.00	25.06
	752	CA	LYS A	A 108	12.422	21.280	11.157	1.00	24.60
	753	CB	LYS A	A 108	13.665	21.628	11.975	1.00	19.20
	754	CG	LYS A	A 108	14.972	21.164	11.350	1.00	17.42
	755	CD	LYS A	A 108	16.158	21.849	12.020	1.00	18.52
30	756	CE	LYS A	108	17.488	21.171	11.715	1.00	23.17
	757	NZ	LYS A	108	17.816	21.133	10.267	1.00	26.96
	758	С	LYS A	108	12.325	19.771	10.976	1.00	28.32
	759	0	LYS A	108	11.738	19.079	11.808	1.00	32.57
	760	N	ILE A	109	12.882	19.252	9.892	1.00	29.02
35	761	CA	ILE F	109	12.797	17.819	9.668	1.00	29.85
	762	СВ	ILE A	109	11.940	17.492	8.406	1.00	29.54
	763	CG2	ILE F	109	11.773	15.980	8.268	1.00	24.76
	764	CG1	ILE F	109	10.557	18.139	8.519	1.00	26.25
	765	CD1	ILE A	109	9.602	17.740	7.412	1.00	26.43
40	766	С	ILE A	109	14.171	17.176	9.530	1.00	31.25
	767	Ö	ILE A	109	15.019	17.653	8.775	1.00	31.58
	768	N	GLN A	110	14.383	16.099	10.283	1.00	34.94
	769	CA	GLN A	110	15.636	15.360	10.254	1.00	35.94

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	770	СВ	GLN	A	110		16.491	15.699	11.472	1.00	43.90
	771	CG	GLN	A	110		16.579	17.182	11.769	1.00	52.49
	772	CD	GLN	Α	110		17.578	17.513	12.860	1.00	53.12
	773	OE1	GLN	Α	110		17.710	18.673	13.266	1.00	42.83
5	774	NE2	GLN	A	110		18.298	16.496	13.338	1.00	66.31
	775	C	GLN	A	110		15.264	13.892	10.293	1.00	35.02
	776	0	GLN	A	110		14.195	13.534	10.792	1.00	36.09
	777	N	MET	Α	111		16.135	13.044	9.762	1.00	34.95
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10	779	CB	MET	A	111		15.299	11.184	8.401	1.00	54.75
	780	CG	MET	A	111		16.107	11.572	7.159	1.00	63.44
	781	SD	MET	A	111		17.262	10.296	6.580	1.00	75.55
	782	CE	MET	A	111		16.222	8.800	6.651	1.00	63.96
	783	С	MET	Α	111		17.137	10.816	10.093	1.00	39.52
15	784	0	MET	A	111		18.190	11.030	9.501	1.00	42.08
	785	N .	ILE	A	112		17.018	9.903	11.057	1.00	39.74
	786	CA	ILE	A	112		18.140	9.069	11.494	1.00	38.26
	787	СВ	ILE	A	112		18.291	9.077	13.030	1.00	37.80
	788	CG2	ILE	A	112		18.536	10.490	13.526	1.00	34.53
20	789	CG1	ILE	A	112		17.039	8.470	13.667	1.00	42.15
ť	790	CD1	ILE	A	112		17.143	8.260	15.149	1.00	40.41
	791	С	ILE	A	112		17.978	7.612	11.078	1.00	33.52
	792	0	ILE	A	112		16.862	7.104	10.969	1.00	28.71
	793	N	GLY	A	113		19.104	6.943	10.860	1.00	30.89
25	794	CA	GLY	A	113		19.061	5.547	10.485	1.00	37.18
	795	С	GLY	A	113		19.963	5.229	9.322	1.00	39.38
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	797	N	GLU	A	114		19.994	3.954	8.944	1.00	42.25
	798	CA	GLU	A	114		20.802	3.489	7.826	1.00	50.83
30	799	CB	GLU	A	114		20.946	1.961	7.878	1.00	64.49
	800	CG	GLU	A	114		21.957	1.446	8.913	1.00	73.99
	801	CD	GLU				21.327	0.579	9.988	1.00	75.69
	802		GLU				20.709	1.131	10.927	1.00	75.15
	803	OE2	GLU	A	114		21.449	-0.661	9.888	1.00	71.34
35		С	GLU	A	114		20.102	3.923	6.542	1.00	55.84
	805	0	GLU	Α	114		19.401	3.148	5.895	1.00	57.72
	806	N	THR	A	115		20.311	5.183	6.189	1.00	57.14
	807	CA	THR	A	115		19.697	5.786	5.017	1.00	58.68
	808	CB	THR				19.866	7.297	5.065	1.00	53.84
40	809		THR				21.235		4.805	1.00	53.59
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	813	N	ASP A	116	21.186	4.363	3.713	1.00	67.68
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	820	0	ASP A	116	21.426	2.430	0.614	1.00	76.40
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	902	CD	2 LEU	A 126	11.8	03 11.764	5.167	1.00	22.64
5	903	С	LEU	A 126	14.6	50 14.306	2.900	1.00	39.09
	904	0.	LEU	A 126	14.6	44 15.313	3.595	1.00	41.65
	905	N	THR	A 127	15.6	52 13.998	2.097	1.00	36.98
	906	CA	THR	A 127	16.8	10 14.864	1.971	1.00	42.37
	907	СВ	THR	A 127	17.6	77 14.406	0.801	1.00	49.56
- 10	908	OG	1 THR	A 127	18.0	86 13.050	1.023	1.00	47.49
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	910	С	THR	A 127	16.3	52 16.299	1.726	1.00	46.79
	911	0	THR	A 127	16.78	87 17.232	2.405	1.00	50.37
	912	N	LYS	A 128	15.4	63 16.456	0.749	1.00	49.56
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	916	CD	LYS .	A 128	14.19	93 16.722	-3.211	1.00	60.97
	917	CE	LYS :	A 128	12.71	13 16.978	-3.451	1.00	65.54
20	918	NZ	LYS 2	A 128	12.07	70 15.978	-4.364	1.00	64.13
	919	С	LYS I	A 128	14.12	26 18.376	1.531	1.00	45.28
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	921	N	ALA A	A 129	13.16	17.635	2.073	1.00	45.11
	922	CA	ALA A	A 129	12.35	9 18.145	3.177	1.00	46.45
25.	923	CB	ALA A	129	11.41	17.068	3.665	1.00	49.46
	924	С	ALA A	129	13.22	9 18.634	4.332	1.00	44.27
	925	0	ALA A	129	12.80	0 19.463	5.132	1.00	41.06
	926	N	GLU F	130	14.44	5 18.099	4.418	1.00	44.20
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30	928	CB	GLU A	130	16.49	4 17.442	5.599	1.00	44.22
	929	CG		130	16.00	6 16.064	6.000	1.00	49.59
	930	CD	GLU A		17.14	2 15.111	6.324	1.00	49.64
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	941	OE2	GLU A	131	20.25	l 21.699	2.529	1.00	67.98

	942	C.	GLU	J	131		15.954	22.179	3.170	1.00	39.85
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	944	N	LEU	J	132		14.671	21.957	2.926	1.00	40.81
	945	CA	LEU	ĮĮ	132		13.686	23.023	3.008	1.00	40.93
5	946	CB	LEU	Į	132		12.303	22.480	2.631	1.00	42.02
	947	CG	LEU	J P	132		11.104	23.429	2.735	1.00	37.20
	948	CD:	1 LEU	<i>p</i>	132	•	11.372	24.670	1.914	1.00	40.73
	949	CD:	2 LEU	A	132		9.840	22.736	2.246	1.00	22.65
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10	951	0	LEU	A	132		13.697	24.845	4.565	1.00	37.40
	952	N	THR	A	133		13.533	22.767	5.404	1.00	43.53
	953	CA	THR	. A	133		13.416	23.187	6.797	1.00	43.29
	954	CB	THR	A	133		12.535	22.179	7.565	1.00	30.42
	955	OG1	LTHR	A	133		12.944	20.842	7.242	1.00	32.09
15	956	CG2	THR	A	133		11.076	22.353	7.178	1.00	29.55
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25	966	С	LYS	A	134			24.715	8.751	1.00	44.36
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	968	N			135		16.905	25.958	8.303	1.00	49.25
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35	976	N			136		14.754	26.213	10.099		51.08
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                                                 19.894
     1137
            CD1 LEU A 157
                                30.382
                                        -1.459 20.970 1.00 66.20
25
     1138
            CD2 LEU A 157
                                31.992
                                        -1.869
                                                19.058
                                                         1.00 73.25
     1139
            С
                LEU A 157
                                32.082
                                         0.921
                                                17.349 1.00 53.24
     1140
            0
                LEU A 157
                                33.220
                                         0.654
                                                17.728
                                                         1.00 53.64
     1141
                LYS A 158
                                31.725
                                         0.912
                                                16.071
                                                         1.00 48.90
     1142
            CA
                LYS A 158
                                32.656
                                         0.571 15.003
                                                         1.00 43.03
30
     1143
            CB
                LYS A 158
                                31.868
                                         0.042
                                                13.799
                                                         1.00 51.76
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            CG
                LYS A 158
                               32.699
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                                                         1.00 50.73
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           CD
                LYS A 158
                                        -1.683
                                31.946
                                                11.978
                                                        1.00 59.64
     1146
           CE
                LYS A 158
                               30.530
                                        -1.275
                                                11.550
                                                        1.00 62.25
     1147
           NZ
                LYS A 158
                               29.722
                                        -2.409
                                                10.995
                                                         1.00 58.23
35
     1148
           С
                LYS A 158
                               33.470
                                         1.807
                                                14.621
                                                        1.00 38.44
     1149
           0
                LYS A 158
                               34.691
                                         1.745
                                                14.521
                                                        1.00 36.00
     1150
           Ν
                LEU A 159
                               32.782
                                         2.928
                                                14.415
                                                        1.00 39.17
     1151
           CA
                LEU A 159
                               33.427
                                         4.193
                                                14.067
                                                        1.00 39.21
     1152
           СВ
                LEU A 159
                               32.393
                                         5.317
                                                14.005
                                                        1.00 46.03
40
     1153
           CG
                LEU A 159
                               31.495
                                         5.432
                                                12.778
                                                        1.00 49.65
     1154
           CD1 LEU A 159
                               30.339
                                         6.380
                                                13.064
                                                        1.00 52.44
     1155
           CD2 LEU A 159
                               32.322
                                         5.929
                                                11.611
                                                        1.00 50.53
     1156
           С
                LEU A 159
                               34.487
                                         4.570
                                                15.097
                                                        1.00 38.04
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	1157	0	LEU	J A	159	35.552	5.070	14.745	1.00	32.72
	1158	N	ILE	A	160	34.180	4.346	16.372	1.00	39.18
	1159	CA	ILE	: A	160	35.110	4.661	17.451	1.00	39.26
	1160	СВ	ILE	A	160	34.451	4.464	18.828	1.00	29.65
5	1161	CG2	2 ILE	A	160	35.467	4.701	19.939	1.00	21.54
	1162	CG1	LILE	A	160	33.274	5.424	18.981	1.00	33.17
	1163	CDI	LILE	: A	160	32.497	5.216	20.252	1.00	27.59
	1164	С	ILE	A	160	36.346	3.768	17.358	1.00	42.75
	1165	0	ILE	Α	160	37.472	4.253	17.404	1.00	41.60
. 10	1166	N	SER	A	161	36.138	2.463	17.224	1.00	47.98
	1167	CA	SER	A	161	37.261	1.539	17.113	1.00	52.98
	1168	СВ	SER	A	161	36.779	0.087	17.167	1.00	51.83
	1169	OG	SER	Α	161	36.293	-0.244	18.457	1.00	47.45
	1170	С	SER	A	161	37.998	1.778	15.805	1.00	54.93
15	1171	0	SER	A	161	38.787	0.945	15.366	1.00	59.36
	1172	N	GLN	Α	162	37.722	2.915	15.177	1.00	54.75
	1173	CA	GLN	Α	162	38.367	3.277	13.927	1.00	57.55
	1174	СВ	GLN	Α	162	37.323	3.550	12.849	1.00	57.42
	1175	·CG	GLN	A	162	37.917	3.877	11.489	1.00	59.30
20	1176	CD	GLN	A	162	38.609	2.687	10.859	1.00	61.11
	1177	OE1	GLN	A	162	39.542	2.125	11.427	1.00	65.88
	1178	NE2	GLN	A	162	38.152	2.296	9.676	1.00	72.94
	1179	С	GLN	Α	162	39.194	4.530	14.176	1.00	60.23
	1180	0	GLN	Α	162	40.353	4.614	13.776	1.00	61.01
25	1181	N	ASP	A	163	38.587	5.507	14.839	1.00	61.53
	1182	CA	ASP	A	163	39.277	6.745	15.166	1.00	59.20
	1183	CB	ASP	A	163	38.298	7.743	15.792	1.00	59.79
	1184	CG	ASP	A	163	37.203	8.170	14.834	1.00	63.02
	1185	OD1	ASP	A	163	36.632	7.292	14.158	1.00	72.81
30	1186	OD2	ASP	A	163	36.904	9.380	14.762	1.00	61.86
	1187	С	ASP	A	163	40.388	6.400	16.159	1.00	57.70
	1188	0	ASP	A	163	41.429	7.051	16.193	1.00	55.82
	1189	N	VAL	A	164	40.151	5.367	16.963	1.00	57.73
	1190	CA	VAL	A	164	41.119	4.914	17.953	1.00	59.37
35	1191	CB	VAL	Α	164	40.519	3.862	18.891	1.00	55.59
	1192	CG1	VAL	A	164	41.604	3.296	19,801	1.00	47.40
	1193	CG2	VAL	A	164	39.416	4.479	19.714	1.00	51.18
	1194	С	VAL	A	164	42.286	4.270	17.242	1.00	62.08
	1195	0	VAL	A	164	43.447	4.509	17.573	1.00	65.19
40	1196	N	LEU	A	165	41.963		16.268	1.00	63.92
	1197	CA	LEU			42.978		15.490	1.00	62.86
	1198	CB	LEU	A	165	42.311	1.737	14.555	1.00	45.47
	1199	CG	LEU	Α	165	43.218	0.747	13.834	1.00	40.70

	1200	CD1	LEU.	Α	165		42.521	-0.595	13.698	1.00	39.99
	1201	CD2	LEU	A	165		43.592	1.318	12.485	1.00	39.90
	1202	C	LEU	A	165		43.750	3.796	14.704	1.00	63.35
	1203	0	LEU	Α	165		44.981	3.788	14.683	1.00	63.16
5	1204	N	ASP	A'	166		43.020	4.713	14.076	1.00	64.85
	1205	CA	ASP	A	166		43.634	5.793	13.312	1.00	65.80
	1206	СВ	ASP	А	166		42.581	6.521	12.477	1.00	71.82
	1207	CG	ASP	Α	166		42.153	5.728	.11.263	1.00	70.86
	1208	OD1	ASP	A	166		41.740	4.561	11.428	1.00	65.25
10	1209	OD2	ASP	Α	166		42.227	6.272	10.141	1.00	80.37
	1210	С	ASP	А	166		44.298	6.781	14.265	1.00	66.21
	1211	0	ASP	Α	166		44.567	7.927	13.903	1.00	65.89
•	1212	N	ALA	A	167		44.552	6.323	15.488	1.00	66.17
	1213	CA	ALA	Α	167		45.185	7.138	16.519	1.00	66.51
15	1214	СВ	ALA	Α	167		46.691	7.204	16.277	1.00	63.12
	1215	С	ALA	Α	167		44.602	8.547	16.600	1.00	67.20
	1216	0	ALA	Α	167		45.170	9.499	16,067	1.00	64.87
	1217	N	LYS	Α	168		43.457	8.666	17.264	1.00	69.56
	1218	CA	LYS	A	168		42.800	9.954	17.444	1.00	70.73
20	1219	CB	LYS	Α	168		41.515	10.034	16.629	1.00	55.74
	1220	CG	LYS	A	168		41.739	10.195	15.158	1.00	43.98
	1221	CD	LYS	A	168		40.450	10.600	14.486	1.00	50.77
	1222	CE	LYS	A	168		40.682	10.922	13.021	1.00	54.71
	1223	NZ	LYS	Α	168	i k	41.325	9.779	12.312	1.00	56.54
25	1224	С	LYS	Α	168		42.466	10.129	18.909	1.00	74.61
	1225	0	LYS	A	168	,	42.990	11.020	19.580	1.00	79.29
	1226	N	ILE	A	169		41.583	9.272	19.401	1.00	75.01
	1227	CA	ILE	Α	169		41.196	9.325	20.795	1.00	77.20
	1228	СВ	ILE	A	169		39.651	9.321	20,960	1.00	70.32
30	1229	CG2	ILE	A	169	•	39.053	10.497	20.203	1.00	64.44
	1230	CG1	ILE	A	169		39.049	8.011	20.444	1.00	67.21
	1231	CD1	ILE	A	169		39.169	7.812	18.957	1.00	62.39
	1232	С	ILE	A	169		41.805	8.112	21.478	1.00	81.65
	1233	0	ILE	A	169		41.777	7.008	20.933	1.00	82.71
35	1234	N	ASN	A	170		42.384	8.328	22.656	1.00	84.48
	1235	CA	ASN	A	170		43.003	7.240	23.402	1.00	86.01
	1236	СВ	ASN	A	170		43.440	7.699	24.803	1.00	99.20
	1237	CG	ASN	A	170		44.062	9.090	24.809	1.001	.05.24
	1238	OD1	ASN	Α	170		44.731	9.491	23.855	1.001	.09.37
40	1239	ND2	ASN	A	170		43.856	9.826	25.900	1.001	.04.96
	1240	, C	ASN	A	170		41.951	6.162	23.551	1.00	84.21
	1241	0	ASN	A	170		40.761	6.458	23.611	1.00	83.04
	1242	N	PRO	A	171		42.364	4.892	23.600	1.00	84.49

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	1243	CD	PRO	A	171	43.716	4.318	23.698	1.00	86.08
	1244	CA	PRO	Α	171	41.335	3.862	23.753	1.00	84.63
	1245	СВ	PRO	A	171	42.141	2.567	23.713	1.00	86.37
	1246	CG	PRÓ	Α	171	43.442	2.977	24.344	1.00	86.68
5	1247	С	PRO	À	171	40.643	4.094	25.097	1.00	82.79
	1248	0	PRO	A	171	39.598	3.513	25.392	1.00	82.76
	1249	N	GLY	Α	172	41.246	4.969	25.898	1.00	80.64
	1250	CA	GLY	A	172	40.703	5.297	27.201	1.00	81.32
	1251	С	GLY	Α	172	39.764	6.488	27.163	1.00	81.29
10	1252	0	GLY	Ā	172	39.094	6.783	28.151	1.00	83.71
	1253	N	ASP	Α	173	39.721	7.182	26.030	1.00	79.07
	1254	CA	ASP	Α	173	38.842	8,336	25.870	1.00	75.74
	1255	СВ	ASP	Α	173	39.260	9.159	24.651	1.00	85.90
	1256	CG	ASP	A	173	40.356	10.146	24.968	1.00	90.56
15	1257	OD1	ASP	. A	173	41.327	9.754	25.645	1.00	93.25
	1258	OD2	AȘP	Α	173	40.248	11.313	24.536	1.00	92.57
	1259	C	ASP	A	173	37.393	7.884	25.711	1.00	70.25
	1260	0	ASP	A	173	36.464	8.691	25.777	1.00	68.50
	1261	N	ILE	A	174	37.207	6.587	25.495	1.00	65.51
20	1262	CA	ILE	Α	174	35.876	6.023	25.340	1.00	60.45
	1263	СВ	ILE	A	174	35.956	4.517	25.071	1.00	48.40
	1264	CG2	ILE	A	174	34.564	3.936	24.911	1.00	46.12
	1265	CG1	ILE	A	174.	36.789	4.274	23.815	1.00	44.86
	1266	CD1	ILE	A	174	37.028	2.817	23.515	1.00	31.07
25	1267	С	ILE	A	174 .	35.086	6.256	26.621	1.00	58.37
	1268	0	ILE	A	174	35.421	5.712	27.668	1.00	58.27
	1269	N	THR	A	175	34.042	7.071	26.535	1.00	55.65
	1270	CA	THR	A	175	33.210	7.371	27.691	1.00	53.67
	.1271	CB	THR	A	175	33.526	8.765	28.240	1.00	57.15
30	1272	OG1	THR	A	175	33.103	9.758	27.300	1.00	55.78
	1273	CG2	THR	A	175	35.012	8.915	28.453	1.00	49.80
	1274	С	THR	A	175	31.751	7.336	27.264	1.00	52.38
	1275	0	THR	A	175	31.454	7.143	26.089	1.00	52.43
	1276	N	GLU	Α	176	30.835	7.512	28.208	1.00	51.31
35	1277	CA	GLU	A	176	29.423	7.518	27.858	1.00	48.46
	1278	CB	GLU	A	176 ·	28.555	7.471	29.114	1.00	37.51
	1279	CG	GLU	A	176	28.426	6.080	29.688	1.00	45.01
	1280	CD	GLU	A	176	27.472	6.010	30.858	1.00	45.89
	1281					26.435	6.716	30.834	1.00	42.92
40	1282	OE2	GLU	A	176	27.757	5.231	31.792	1.00	34.90
	1283	C	GLU	A	176	29.130	8.777	27.056	1.00	49.50
	1284	0	GLU	A	176	28.255	8.793	26.192	1.00	49.76
	1285	N	GLU	A	177	29.879	9.833	27.349	1.00	48.42

	1286	CA	GLU	A	177	29.721	11.092	26.645	1.00	48.94
	1287	СВ	GLU	A	177	30.646	12.153	27.253	1.00	63.07
	1288	CG	GLU	A	177	30.554	13.528	26.589	1.00	72.68
	1289	CD	GLU	A	177	31.888	14.267	26.554	1.00	76.09
5	1290	OE1	GLU	Α	177	31.912	15.439	26.114	1.00	77.97
	1291	OE2	GLU	A	177	32.914	13.675	26.957	1.00	76.21
	1292	С	GLU	A	177	30.095	10.867	25.179	1.00	47.13
	1293	0	GLU	A	177	29.340	11.210	24.269	1.00	43.82
	1294	N	LEU	Α	178	31.266	10.274	24.964	1.00	46.13
10	1295	CA	LEU	A	178	31.774	10.012	23.620	1.00	41.18
	1296	CB	LEU	A	178	33.167	9.373	23.704	1.00	31.24
	1297	CG	LEU	A	178	33.980	9.227	22.411	1.00	29.48
	1298	CD1	LEU	Α	178	35.389	8.792	22.756	1.00	32.21
	1299	CD2	LEU	A	178	33.344	8.213	21.481	1.00	38.13
15	1300	С	LEU	A	178	30.839	9.128	22.800	1.00	41.26
	1301	0	LEU	A	178	30.355	9.551	21.752	1.00	44.23
	1302	N	ILE	Α	179	30.596	7.905	23.271	1.00	37.47
·	1303	CA	ILE	A	179	29.716	6.967	22.573	1.00	33.95
	1304	CB	ILE	Α	179	29.324	5.780	23.479	1.00	25.86
20	1305	CG2	ILE	A	179	28.262	4.950	22.807	1.00	27.50
	1306	CG1	ILE	A	179	30.545	4.905	23.762	1.00	24.58
	1307	CD1	ILE	A	179	30.292	3.777	24.748	1.00	16.92
	1308	С	ILE	A	179	28.443	7.673	22.127	1.00	36.09
	1309	0	ILE	A	179	27.885	7.374	21.069	1.00	36.52
25	1310	N	GLY	A	180	27.997	8.622	22.944	1.00	37.19
• •	1311	CA	GLY	A	180	26.792	9.370	22.639	1.00	34.45
	1312	С	GĻY	Α	180	26.935	10.318	21.466	1.00	33.00
	1313	0	GLY	A	180	25.951	10.639	20.794	1.00	32.59
	1314	N	ASN	A	181	28.157	10.777	21.222	1.00	35.65
30	1315	CA	ASN	A	181	28.411	11.687	20.114	1.00	34.95
	1316	CB	ASN	A	181.	29.701	12.475	20.339	1.00	30.99
	1317	CG	ASN	A	181	29.654	13.321	21.578	1.00	27.11
	1318	OD1	ASN	A	181	28.679	14.027	21.818	1.00	30.62
	1319	ND2	ASN	A	181	30.715	13.268	22.372	1.00	34.99
35	1320	С	ASN	A	181	28.528	10.929	18.804	1.00	32.99
	1321	0	ASN	A	181	28.625	11.546	17.751	1.00	27.15
	1322	N	TYR	A	182	28.523	9.599	18.868	1.00	31.98
	1323	CA	TYR	A	182	28.645	8.778	17.670	1.00	30.09
	1324	CB	TYR	A	182	29.708	7.712	17.869	1.00	29.07
40	1325	CG	TYR			31.121	8.224	17.726	1.00	30.62
	1326	CD1	TYR	A	182	31.630	9.198	18.589	1.00	31.56
	1327	CE1	TYR	A	182	32.954	9.652	18.467	1.00	31.15
	1328	CD2	TYR	A	182	31.965	7.715	16.735	1.00	32.17

	1329	CE	2 TYR A	182	33.287	8.156	16.606	1.00	29.49
	1330	CZ	TYR A	182	33.774	9.123	17.473	1.00	30.88
	1331	ОН	TYR A	182	35.079	9.548	17.337	1.00	38.87
	1332	С	TYR A	182	27.353	8.116	17.247	1.00	30.63
5	1333	0	TYR A	182	27.316	7.417	16.238	1.00	27.81
	1334	N	LEU A	183	26.296	8.331	18.023	1.00	33.68
	1335	CA	LEU A	183	24.987	7.764	17.712	1.00	39.37
	1336	СВ	LEU A	183	24.169	7.618	18.995	1.00	39.69
	1337	CG	LEU A	183	24.813	6.778	20.096	1.00	35.29
. 10	1338	CD	LEU A	183	23.932	6.801	21.332	1.00	30.83
	1339	CD2	2 LEU A	183	25.016	5.361	19.602	1.00	36.26
	1340	С	LEU A	183	24.250	8.671	16.715	1.00	40.34
	1341	0	LEU A	183	24.537	9.865	16.626	1.00	39.87
	1342	N	PHE A	184	23.302	8.110	15.969	1.00	38.84
15	1343	CA	PHE A	184	22.556	8.890	14.984	1.00	37.83
	1344	СВ	PHE A	184	21.432	8.058	14.354	1.00	31.19
	1345	CG	PHE A	184	21.894	6.766	13.729	1.00	28.22
	1346	CD1	PHE A	184	23.182	6.633	13.229	1.00	30.85
	1347	CD2	PHE A	184	21.019	5.687	13.616	1.00	33.99
20	1348	CE1	PHE A	184	23.587	5.443	12.627	1.00	24.17
	1349	CE2	PHE A	184	21.417	4.493	13.013	1.00	21.76
	1350	CZ	PHE A	184	22.699	4.372	12.519	1.00	18.36
	1351	С	PHE A 1	184	21.952	10.145	15.604	1.00	36.97
	1352	0	PHE A 1	184	21.698	11.130	14.912	1.00	32.04
25	1353	N	THR A 1	L85	21.719	10.104	16.909	1.00	38.47
	1354	CA	THR A 1	185	21.145	11.244	17.609	1:00	42.41
	1355	CB	THR A 1		20.396	10.787	18.846	1.00	34.61
	1356		THR A 1		21.213	9.862	19.570	1.00	41.28
20	1357		THR A 1	.85	19.104	10.116	18.454		34.33
30	1358	С	THR A 1			12.254		1.00	44.70
	1359	0	THR A 1			13.086	18.905	1.00	41.53
	1360	N	GLN A 1		23.374	12.179	17.413	1.00	48.74
	1361	CA	GLN A 1		24.494	13.072	17.711	1.00	49.59
25	1362	CB	GLN A 1		25.775	12.501	17.132	1.00	45.10
35	1363	CG	GLN A 1		25.837	12.676	15.628	1.00	43.93
	1364	CD	GLN A 1		27.074	12.068	15.013	1.00	47.95
	1365		GLN A 1		27.201	10.848	14.920	1.00	50.02
	1366		GLN A 1		28.000	12.918	14.593	1.00	38.99
40	1367	С	GLN A 1		24.279	14.451	17.097		51.53
40	1368	0	GLN A 1		25.031	15.389	17.370		55.42
	1369	N	HIS A 1		23.262	14.555	16.249		50.40
	1370	CA	HIS A 1		22.934		15.568		49.57
	1371	CB	HIS A 1	87	22.157	15.474	14.295	1.00	42.89

	1372	CG	HIS	A	187		22.856	14.473	13.427	1.00	49.91
	1373	CD2	HIS	A	187		22.458	13.268	12.951	1.00	49.67
	1374	· ND1	HIS	A	187		24.159	14.638	13.006	1.00	43.80
	1375	CE1	HIS.	A	1.87		24.536	13.578	12.311	1.00	48.87
5	1376	NE2	HIS	A	187		23.523	12.731	12.263	1.00	46.70
	1377	С	HIS	A	187		22.145	16.735	16.469	1.00	52.33
	1378	0	HIS	A	187		22.402	17.936	16.513	1.00	53.97
	1379	N	LEU	A	188		21.187	16.182	17.196	1.00	54.52
	1380	CA	LEU	A	188	1	20.391	16.982	18.109	1.00	51.83
10	1381	CB	LEU	A	188		19.256	16.127	18.682	1.00	44.55
	1382	CG	LEU'	A	188		18.288	15.528	17.650	1.00	47.65
	1383	CD1	LEU	Α	188		17.311	14.577	18.332	1.00	49.93
	1384	CD2	LEU	A	188		17.539	16.645	16.937	1.00	56.89
	1385	С	LEU	Α	188		21.309	17.487	19.229	1.00	52.44
15	1386	0	LEU	A	188		22.248	16.802		1.00	53.35
	1387	N	PRO	A	189		21.056	18.700	19.738	1.00	51.33
	1388	CD	PRO	A	189		19.887	19.538	19.434	1.00	51.94
	1389	CA	PRO	Α	189		21.858	19.302	20.815	1.00	49.93
	1390	CB	PRO	A	189	٠.	21.115	20.601	21.115	1.00	51.02
20	1391	CG	PRO	A	189	٠	19.701	20.275	20.733	1.00	52.36
	1392	С	PRO	A	189		21.978	18.411	22.045	1.00	46.59
	1393	0	PRO				21.001	17.807	22.476	1.00	45.97
	1394	N			190		23.169	18.351	22.625		42.50
05		CA			190		23.390		23.782		39.80
25	1396	СВ	LŸS		· .		24.672		24.526	1.00	36.33
	1397	CG	LYS				25.964	17.462			38.65
	1398	CD	LYS				27.169	17.626			42.37
	1399	CE	LYS				28.493	17.455	,		50.39
20	1400	NZ	LYS				28.687	16.085			58.82
30	1401	C	LYS				22.256		24.789		
	1402	0	LYS				21.827		25.075		
	1403	N Ch	ASP				21.751	18.475	25.328		40.10
	1404	CA	ASP				20.687	18.345	26.323		39.42
35	1405 1406	CB	ASP				20.538	19.644			39.52
33	1400	CG OD1	ASP				20.012	20.819	26.328		44.32
	1407		ASP .				20.747	21.289	25.429		39.96
	1400	C	ASP				18.866	21.275	26.589		42.53
	1410	0	ASP .				19.323	17.893	25.777		39.16
40	1411	N					18.378				41.35
10		CA	LEU .				19.223		24.460		37.21
	1413	CB	LEU .				17.962		23.850		34.43
	1414	CG	LEU .				17.484	18.337	22.815		26.76
	TATA	CG	neO ,	C,	192		16.902	19.649	23.372	1.00	23.82

	1415	CD	1 LEU A 192	16.704	20.638	22.253	1.00 16.92
	1416	CD	2 LEU A 192	15.570	19.379	24.088	1.00 16.92
	1417	С	LEU A 192	18.039	15.911	23.203	1.00 34.24
	1418	0	LEU A 192	17.031	15.380	22.746	1.00 38.50
5	1419	N	ARG A 193	19.235	15.328	23.193	1.00 30.50
	1420	CA	ARG A 193	19.469	14.016	22.598	1.00 29.14
	1421	СВ	ARG A 193	20.949	13.650	22.679	1.00 23.71
	1422	CG	ARG A 193	21.825	14.473	21.795	1.00 24.21
	1423	CD	ARG A 193	23.274	14.087	21.962	1.00 20.84
10	1424	NE	ARG A 193	24.139	14.813	21.033	1.00 31.16
	1425	CZ	ARG A 193	25.463	14.694	20.994	1.00 37.18
	1426	NH:	1 ARG A 193	26.087	13,874	21.837	1.00 39.87
	1427	NH2	2 ARG A 193	26.163	15.390	20.107	1.00 37.17
	1428	С	ARG A 193	18.670	12.853	23.166	1.00 28.97
15	1429	0	ARG A 193	18.305	11.949	22,427	1.00 29.31
	1430	N	ASP A 194	18.399	12.846	24.463	1.00 24.43
	1431	CA	ASP A 194	17.665	11.723	25.024	1.00 26.20
	1432	CB	ASP A 194	18.295	11.282	26.354	1.00 21.25
	1433	CG	ASP A 194		10.856	26.208	1.00 25.14
20	1434		ASP A 194		10.315	25.138	1.00 16.92
	1435		2 ASP A 194	20.543	11.047	27.175	1.00 30.59
	1436	С	ASP A 194	16.187	12.025	25.228	1.00 24.70
	1437	, 0	ASP A 194	15.826	13.067	25.776	1.00 31.23
٥٣	1438	N	PRO A 195	15.309	11.110	24.784	1.00 19.04
25	1439	CD	PRO A 195		9.811	24.159	1.00 16.92
	1440	CA	PRO A 195	13.865	11.293	24.929	1.00 22.28
	1441	CB	PRO A 195	13.290	10.066	24.231	1.00 21.56
	1442	CG	PRO A 195	14.334	9.050	24.426	1.00 18.86
20	1443	С	PRO A 195	13.490	11.347	26.391	1.00 24.96
30	1444	0	PRO A 195	14.092	10.660	27.206	1.00 30.51
	1445	N	ASP A 196	12.510	12.172		1.00 22.33
	1446	CA	ASP A 196	12.081	12.284	28.112	
	1447	CB	ASP A 196	11.799	13.737	28.464	1.00 21.17
35	1448	CG	ASP A 196	13.024	14.589	28.347	1.00 35.32
55	1449		ASP A 196	13.290	15.099	27.239	1.00 31.80
	1450 1451	C	ASP A 196	13.739	14.725	29.361	1.00 44.56
	1451	0	ASP A 196		11.437	28.336	1.00 22.00
	1452	N	ASP A 196		11.258	29.461	1.00 22.34
40			LEU A 197		10.910	27.239	1.00 24.46
10	1454 1455	CA	LEU A 197		10.063	27.283	1.00 22.14
	1455	CB	LEU A 197 LEU A 197		10.900	27.460	1.00 16.92
					10.182	27.174	1.00 16.92
	1457	CDI	LEU A 197	6.452	8.939	28.004	1.00 18.26

	1458	CD2	LEU	A	197	5.424	11.093	27.470	1.00	23.97
	1459	С	LEU	A	197	9.100	9.292	25.987	1.00	24.32
	1460	0	LEU	A	197	9.396	9.825	24.925	1.00	31.10
	1461	N	ILE	A	198	8.752	8.018	26.082	1.00	25.23
5	1462	CA	ILE	Α	198	8.617	7.198	24.899	1.00	23.49
	1463	СВ	ILE	A	198	9.663	6.079	24.843	1.00	16.92
	1464	CG2	ILE	A	198	9.389	5.176	23.651	1.00	16.92
	1465	CG1	ILE	A	198	11.057	6.698	24.719	1.00	19.52
	1466	CD1	ILE	A	198	12.156	5.717	24.368	1.00	16.92
10	1467	С	ILE	A	198	7.214	6.621	24.894	1.00	26.00
	1468	0	ILE	A	198	6.835	5.840	25.767	1.00	23.12
	1469	N	ILE	A	199	6.448	7.056	23.901	1.00	30.16
	1470	CA	ILE	A	199	5.070	6.649	23.719	1.00	31.89
	1471	CB	ILE	A	199	4.275	7.798	23.061	1.00	31.40
15	1472	CG2	ILE	A	199	2.850	7.347	22.743	1.00	35.99
	1473	CG1	ILE	A	199	4.300	9.019	23.991	1.00	30.96
	1474	CD1	ILE	A	199	3.589	10.238	23.458	1.00	25.50
•	1475	С	ILE	A	199	4.976	5.393	22.859	1.00	30.27
	1476	0	ILE	A	199	5.705	5.249	21.881	1.00	30.43
20	1477	N	ARG	A	200	4.087	4.483	23.246	1.00	29.84
	1478	CA	ARG	A	200	3.868	3.240	22.513	1.00	34.70
	1479	CB	ARG	A	200	4.567	2.070	23.214	1.00	38.24
	1480	CG	ARG	A	200	4.553	0.763	22.420	1.00	38.39
	1481	CD	ARG	A	200	5.267	0.900	21.074	1.00	41.65
25	1482	NE	ARG	A	200	5.195	-0.302	20.234	1.00	34.53
•	1483	CZ	ARG	A	200	5.923	-1.409	20.400	1.00	18.77
	1484				200	6.807	-1.510	21.385	1.00	16.92
	1485		ARG			5.771	-2.423	19.566	1.00	18.24
	1486	С			200			22.461		35.76
30	1487		ARG	Α	200	1.688	3.032	23.490	1.00	33.19
	1488				201		2.801		1.00	38.28
	1489	CA			201		2.610			37.05
	1490	CB			201		3.496			16.92
25	1491				201		3.301		1.00	29.17
35	1492	CG2					4.947		1.00	19.67
	1493	С			201		1.174	20.781	1.00	39.68
	1494	0			201	0.844		20.648	1.00	41.56
	1495	N			202	-1.314		20.689	1.00	41.87
40	1496				202	-1.874		20.376	1.00	39.34
40	1497	CB			202	-1.198		19.122		19.15
	1498	OG			202		-2.227			39.12
		C					-1.421			40.05
	1500	0	SER	A	202	-2.303	-2.540	21.280	1.00	47.17

	.,									
	1501	N	GLY	A 203		-1.264	-1.080	22.634	1.00	38.45
	1502	CA	GLY .	A 203		-1.183	-2.038	23.729	1.00	37.08
	1503	С	GLY A	A 203		0.126	-2.815	23.773	1.00	35.70
	1504	0	GLY	A 203		0.305	-3.717	24.591	1.00	37.31
. 5	1505	N	GLU Z	A 204		1.048	-2.459	22.888	1.00	29.52
	1506	CA	GLU Z	A 204		2.336	-3.121	22.824	1.00	28.07
	1507	СВ	GLU Z	A 204	'	3.010	-2.835	21.484	1.00	26.30
	1508	CG	GLU	A 204		2.478	-3.664	20.328	1.00	48.79
	1509	CD	GLU I	A 204	•	2.437	-5.147	20.655	1.00	50.97
10	1510	OE1	GLU	A 204		1.371	-5.628	21.104	1.00	42.50
	1511	OE2	GLU Z	A 204		3.470	-5.829	20.481	1.00	50.61
	1512	С	GLU Z	A 204		3.249	-2.673	.23.942	1.00	29.34
	1513	0	GLU A	A 204		3.611	-1.507	24.014	1.00	34.97
	1514	N	LEU A	A 205		3.626	-3.604	24.811	1.00	24.91
15	1515	CA	LEU	A 205		4.523	-3.307	25.925	1.00	25.98
	1516	CB	LEU A	A 205	,	3.943	-3.875	27.217	1.00	25.92
	1517	. CG	LEU A	A 205		2.570	-3.293	27.561	1.00	23.50
	1518	CD1	LEU A	A 205		1.943	-4.043	28.704	1.00	16.92
	1519	CD2	LEU A	A 205		2.724	-1.837	27.917	1.00	30.67
20	1520	С	LEU A	A 205		5.905	-3.894	25.661	1.00	28.56
	1521	0	LEU A	205		6.494	-4.539	26.515	1.00	29.61
	1522	N	ARG A	206		6.418	-3.675	24.462	1.00	33.33
	1523	CA	ARG A	206		7.725	-4.191	24.108	1.00	37.25
	1524	СВ	ARG A	206	,	7.681	-4.932	22.766	1.00	42.74
25	1525	CG	ARG A	206	100	6.327	-5.519	22.392	1.00	40.30
	1526	CD	ARG A	206		6.381	-6.273	21.057	1.00	44.32
	1527	NE	ARG A	206		6.932	-5.469	19.960	1.00	65.13
	1528	CZ	ARG A	206		6.926	-5.836	18.677	1.00	69.76
	1529	NH1	ARG A	206		6.392	-6.999	18.325	1.00	76.09
30	1530	NH2	ARG A	206		7.452	-5.045	17.741	1.00	74.71
	1531	С	ARG A	206		8.631	-2.991	23.963	1.00	42.39
	1532	0	ARG A	206		8.197	-1.852	24.144	1.00	42.90
	1533	N	LEU A	207		9.888	-3.247	23.625	1.00	44.87
	1534	CA	LEU A	207		10.834	-2.167	23.432	1.00	48.66
35	1535	CB	LEU A	207		12.136	-2.472	24.173	1.00	63.61
	1536	CG	LEU A	207		11.996	-2.330	25.693	1.00	70.49
	1537	CD1	LEU A	207		13.290	-2.729	26.376	1.00	76.92
	1538	CD2	LEU A	207		11.633	-0.885	26.044	1.00	75.21
	1539	С	LEU A	207		11.068	-1.969	21.939	1.00	47.29
40	1540	0	LEU A	207		11.315	-0.849	21.484	1.00	47.01
	1541	N	SER A	208		10.971	-3.060	21.183	1.00	42.15
	1542	CA	SER A	208		11.139	-3.019	19.732	1.00	32.73
	1543	СВ	SER A	208		10.005	-2.214	19.099	1.00	33.90

	1544	OG	SER	A	208		8.755	-2.556	19.666	1.00	24.12
	1545	С	SER	A	208		12.470	-2.441	19.263	1.00	28.39
	1546	0	SER	A	208		12.540	-1.821	18.198	1.00	29.45
	1547	N .	ASN	Α	209		13.516	-2.629	20.064	1.00	26.85
5	1548	CA	ASN	A	209		14.861	-2.162	19.719	1.00	27.50
	1549	CB	ASN	A	209		15.404	-3.045	18.573	1.00	16.92
*	1550	CG	ASN	A	209		16.864	-2.763	18.222	1.00	22.61
	1551	OD1	ASN	A	209		17.693	-2.495	19.087	1.00	26.46
	1552	ND2	ASN	A	209		17.182	-2.857	16.939	1.00	20.95
10	1553	С	ASN	A	209		14.909	-0.675	19.348	1.00	32.21
	1554	0	ASN	Α	209		15.759	-0.241	18.573	1.00	34.11
	1555	N	PHE	A	210		14.006	0.108	19.929	1.00	34.72
	1556	CA	PHE	A	210	•	13.947	1.539	19.638	1.00	30.65
	155,7	CB	PHE	Α	210		12.484	2.000	19.582	1.00	21.62
15	1558	CG	PHE	Α	210		12.309	3.442	19.182	1.00	28.42
	1559	CD1	PHE	A	210		12.788	3.902	17.960	1.00	32.07
	1560	CD2	PHE	A	210		11.650	4.334	20.021	1.00	24.66
	1561	CE1	PHE	A	210		12.614	5.221	17.580	1.00	22.48
	1562	CE2	PHE	A	210		11.471	5.653	19.652	1.00	24.33
20	1563	CZ	PHE	A	210		11.955	6.099	18.427	1.00	18.91
	1564	С	PHE	Α	210		14.708	2.350	20.677	1.00	30.28
	1565	0	PHE	A	210	•	14.456	2.224	21.873	1.00	26.90
	1566	N	LEU	A	211		15.636	3.179	20.202	1.00	31.38
	1567	CA	LEU	A	211		16.460	4.030	21.060	1.00	30.02
25	1568	CB	LEU	A	211		15.703	5.307	21.425	1.00	19.94
	1569	CG	LEU	A	211		15.642	6.415	20.381	1.00	17.90
	1570	CD1	LEU	A	211		15.015	7.668	21.000	1.00	17.79
	1571	CD2	LEU	A	211		17.051	6.710	19.886	1.00	28.12
	1572	С	LEU	A	211		16.940	3.356	22.344	1.00	33.52
30	1573	0	LEU	A	211		16.784	3.899	23.445	1.00	35.70
	1574	N	PRO	A	212		17.559	2.175	22.220	1.00	34.82
	1575	CD	PRO	A	212		18.096	1.603	20.977	1.00	34.05
	1576	CA	PRO	A	212		18.058	1.440	23.384	1.00	31.21
	1577	СВ	PRO	A	212		18.807	0.283	22.748	1.00	30.61
35	1578	CG	PRO	A	212		19.305	0.881	21.473	1.00	33.84
	1579	С	PRO	Α	212		18.941	2.279	24.317	1.00	28.88
	1580	0	PRO	A	212		18.734	2.286	25.529	1.00	28.95
	1581	N	TRP	Α	213		19.911	2.991	23.747	1.00	32.89
	1582	CA	TRP	A	213			3.829	24.525	1.00	34.16
40	1583	СВ	TRP	A	213		22.076		23.699	1.00	36.50
	1584	CG			213				24.377		40.25
	1585	CD2	TRP	A	213	-	24.322	4.679	24.939	1.00	41.82
	1586	CE2	TRP	A	213		24.917	5.856	25.451	1.00	42.56

	1587	CE	3 TRP A 213	25.011	3.463	25.060	1.00 36.15
	1588	CD:	1 TRP A 213	22.944	6.404	24.569	1.00 34.48
	1589	NE:	1 TRP A 213	24.054	6.892	25.212	1.00 35.36
	1590	CZ2	2 TRP A 213	26.170	5.851	26.074	1.00 41.79
5	1591	CZ	3 TRP A 213	26.257	3.459	25.680	1.00 44.66
	1592	CH2	2 TRP A 213	26.823	4.647	26.178	1.00 41.35
	1593	С	TRP A 213	20.210	5.143	25.045	1.00 31.31
	1594	0	TRP A 213	20.111	5.350	26.253	1.00 28.47
	1595	N	GLN A 214	19.814	6.031	24.139	1.00 29.42
· 10	1596	CA	GLN A 214	19.235	7.315	24.526	1.00 27.98
	1597	СВ	GLN A 214	18.794	8.086	23.276	1.00 29.16
	1598	CG	GLN A 214	•			1.00 30.26
	1599	CD	GLN A 214				
1.5	1600		. GLN A 214			20.106	-
15	1601		GLN A 214			21.591	1.00 36.97
	1602	С	GLN A 214			25.484	
	1603	0	GLN A 214			26.395	
	1604	N	GLY A 215		6.153	25.271	1.00 24.50
20	1605	CA	GLY A 215		5.956	26.115	1.00 20.34
20	1606	С	GLY A 215		5.288	27.444	1.00 20.33
	1607	0	GLY A 215		4.974	28.179	1.00 19.80
	1608	N	ALA A 216		5.085	27.761	1.00 16.97
,	1609	CA	ALA A 216		4.435	29.008	1.00 17.93
25	1610	CB C	ALA A 216 ALA A 216		4.772	29.324	1.00 17.20
25	1611 1612	0	ALA A 216	17.160		30.207	1.00 20.59
	1613	N	TYR A 217	16.717		30.912	1.00 23.60
	1614	CA	TYR A 217	16.887 16.033	6.055 6.443	30.442	1.00 24.42 1.00 18.63
	1615	СВ	TYR A 217	16.766		32.533	
30	1616	CG	TYR A 217	18.180	7.000	32.935	1.00 16.92
	1617		TYR A 217	19.248			1.00 16.92
	1618		TYR A 217			32.436	1.00 16.92
	1619		TYR A 217	18.462		34.233	1.00 16.92
	1620	CE2		19.768		34.632	1.00 16.92
35	1621	CZ	TYR A 217		6.423	33.730	1.00 16.92
	1622	OH	TYR A 217	22.103		34.115	1.00 16.92
	1623	С	TYR A 217	14.730	7.134	31.154	1.00 16.92
	1624	0	TYR A 217	14.170		31.910	1.00 16.92
	1625	N	SER A 218	14.235			1.00 16.92
40	1626	CA	SER A 218	13.011		29.502	1.00 16.92
	1627	СВ	SER A 218	12.851	7.259	27.999	1.00 23.90
	1628	OG	SER A 218	14.058		27.330	1.00 36.44
	1629	С	SER A 218	11.762	6.965	30.210	1.00 16.92

	1620	^	CED	, 7 λ	210	11 6	71 5	5.798	30.605	1 00	16.92
	1630 1631	O N			218 219	10.8		7.861			16.92
	1632	CA			219	9.5					24.28
	1633	СВ			219			3.727	31.298		
5	1634	CG			219			0.564			31.57
3	1635	CD			219			0.084	33.790		37.84
	1636				219			0.099	33.964		42.71
	1637		GLU			9.4		3.694	34.658		36.71
	1638	C		,	219			5.704	29.875		30.17
10	1639	0			219	9.3		5.791	28.729	,	36.16
	1640	N			220			5.930	30.188		29.51
	1641	CA			220						24.66
	1642	СВ			220	7.5		3.705	29.192		22.54
	1643	CG			220			3.426	29.170		17.48
15	1644							.940	29.324		23.19
	1645		LEU					3.943	and the second		16.92
	1646	С			220	5.7		3.302	29.378		25.51
	1647	0			220		17 5				27.73
	1648	N			221			6.633			23.31
20	1649	CA	TYR	Α	221			5.782	28.360	1.00	21.83
	1650	СВ	TYR	A	221	3.1	.51 7	.214	27.981	1.00	17.51
	1651	CG	TYR	A	221	1.6	66 7	7.401	27.809	1.00	20.23
	1652	CD1	TYR	Α	221	0.8	07 7	.349	28.904	1.00	25.68
	1653	CE1	ΤΫ́R	A	221	-0.5	81 7	1.476	28.746	1.00	30.87
25	1654	CD2	TYR	Α	221	1.1	13 - 7	.588	26.544	1.00	26.61
	1655	CE2	TYR	A	221	-0.2	73 7	7.713	26.372	1.00	32.18
	1656	CZ	TYR	A	221	-1.1	12 7	.655	27.479	1.00	35.05
	1657	ОН	TYR	A	221	-2.4	75 7	7.762	27.315	1.00	38.11
	1658	С	TYR	A	221	2.9	81 4	1.782	27.353	1.00	22.41
30	1659	0	TYR	A	221	3.3	83 4	.763	26.191	1.00	23.28
	1660	N	PHE	A	222	2.0	66 3	3.932	27.799	1.00	24.60
	1661	CA	PHE	A	222	1.4	85 2	2.956	26.893	1.00	25.33
	1662	CB	PHE	A	222	1.8	39 1	527	27.337	1.00	22.58
	1663	CG	PHE	A	222	3.3	19 1	.222	27.299	1.00	25.69
35	1664	CD1	PHE	A	222	4.1	10 1	390	28.429	1.00	26.52
	1665	CD2	PHE	A	222	3.9	18 0).772	26.127	1.00	30.15
	1666	CE1	PHE	A	222	5.4	73 1	.112	28.393	1.00	25.08
	1667	CE2	PHE	A	222	5.2	81 C	.492	26.084	1.00	36.11
	1668	CZ	PHE	A	222	6.0				1.00	30.23
40	1669	С			222	-0.0					25.48
	1670	.0			222						24.81
	1671	N			223						27.43
	1672	CA	THR	A	223	-1.9	64 3	3.393	25.393	1.00	29.24

	1673	СВ	THR	A 223	-2.255	4.769	24.785	1.00 30.96
	1674	OGI	L THR	A 223	-3.666	4.928	24.634	1.00 38.54
	1675	CG2	THR A	A 223	-1.592	4.908	23.423	1.00 18.62
	1676	С	THR A	A 223	-2.473	2.338	24.449	1.00 31.84
5	1677	0	THR A	A 223	-1.721	1.809	23.645	1.00 30.89
	1678	N	ASP A	A 224	-3.757	2.030	24.544	1.00 36.42
	1679	CA	ASP A	A 224	-4.357	1.032	23.671	1.00 40.14
	1680	СВ	ASP A	A 224	-5.613	0.456	24.324	1.00 41.56
	1681	CG	ASP A	A 224	-5.297	-0.570	25.387	1.00 46.72
10	1682	OD1	ASP A	A 224	-6.215	-0.916	26.160	1.00 43.47
	1683	OD2	ASP A	A 224	-4.137	-1.037	25.441	1.00 54.57
	1684	С	ASP A	224	-4.709	1.610	22.301	1.00 40.48
	1685	0	ASP A	A 224	-4.489	0.968	21.271	1.00 42.72
	1686	N	THR A	A 225	-5.250	2.824	22.293	1.00 37.47
15	1687	CA	THR A	A 225	-5.639	3.470	21.047	1.00 37.52
	1688	СВ	THR A	225	-5.820	5.007	21.223	1.00 32.35
	1689	OG1	THR A	225	-4.654	5.558	21.843	1.00 45.94
	1690	CG2	THR A	225	-7.056	5.316	22.074	1.00 27.82
	1691	С	THR F	225	-4.625	3.211	19.937	1.00 36.64
20	1692	0	THR A	225	-3.412	3.257	20.168	1.00 32.74
	1693	N	LEU A	22.6	-5.143	2.912	18.744	1.00 40.20
	1694	CA	LEU A	226	-4.319	2.649	17.572	1.00 37.95
	.1695	. CB	LEU A	226	-5.147	2.000	16.465	1.00 27.85
	1696	CG	LEU A	226	-5.704	0.614	16.768	1.00 16.92
25	1697	CD1	LEU A	. 226	-4.646	-0.162	17.523	1.00 20.23
	1698	CD2	LEU A		-6.971	0.719	17,595	1.00 16.92
	1699	С	LEU A	226	-3.732	3.955	17.074	1.00 34.39
	1700	0	LEU A		-4.371	4.999	17.151	1.00 33.65
••	1701	N	TRP A		-2.518	3.886	16.545	1.00 27.74
30	1702	CA	TRP A		-1.833		16.084	
	1703			227				1.00 16.92
	1704	CG		227			14.859	1.00 16.92
	1705		TRP A		0.690		15.634	1.00 24.25
25				227		7.907		1.00 21.82
35				227	0.766		17.007	1.00 27.14
	1708				0.383		13.554	1.00 16.92
	1709		TRP A				13.465	1.00 18.37
				227			15.150	1.00 17.65
40			TRP A		1.394		17.424	1.00 22.73
40					1.944	_	16.496	1.00 19.73
		С		227	-2.610		15.211	1.00 29.41
				227		_	15.529	
	1715	N	PRO A	228	-3.185	5.581	14.085	1.00 34.10

	1716	CD	PRO	A	228		-3.065	4.256	13.450	1.00	32.12
	1717	CA	PRO	A	228		-3.938	6.495	13.220	1.00	33.56
	1718	CB	PRO	A	228		-4.498	5.573	12.154	1.00	30.46
•	1719	CG	PRO	Α	228		-3.411	4.568	12.010	1.00	31.06
5	1720	С	PRO	A	228		-5.024	7.232	13.975	1.00	36.50
	1721	O.	PRO	A	228		-5.559	8.224	13.489	1.00	39.78
	1722	N	ASP	A	229		-5.338	6.739	15.170	1.00	38.84
	1723	CA	ASP	A	229		-6.358	7.336	16.024	1.00	37.34
	1724	СВ	ASP	Α	229		-7.158	6.234	16.732	1.00	34.82
10	1725	CG	ASP	A	229		-8.247	5.649	15.864	1.00	34.97
	1726	OD1	ASP	A	229		-8.868	4.651	16.279	1.00	49.11
	1727	OD2	ASP	Α	229		-8.497	6.188	14.771	1.00	48.81
	1728	С	ASP	A	229		-5.743	8.258	17.075	1.00	35.86
	1729	0	ASP	Α	229		-6.459	8.814	17.901	1.00	38.47
15	1730	N	PHE	Α	230		-4.423	8.422	17.043	1.00	31.52
	1731	CA	PHE	A	230		-3.732	9.257	18.026	1.00	29.58
	1732	СВ	PHE	A	230		-2.245	8.877	18.112	1.00	30.24
	1733	CG	PHE	A	230		-1.656	8.990	19.507	1.00	39.74
	1734	CD1	PHE	A	230		-2.055	8.123	20.521	1.00	35.52
20	1735	CD2	PHE	A	230		-0.676	9.937	19.796	1.00	36.37
	1736	CE1	PHE	A	230		-1.482	8.192	21.800	1.00	28.22
	1737	CE2	PHE	A	230		-0.099	10.014	21.068	1.00	28.28
	. 1738	CZ	PHE	A	230		-0.504	9.138	22.068	1.00	28.51
•	1739	C	PHE	A	230		-3.866	10.744	17.709	1.00	31.09
25	1740	0	PHE	A	230		-3.033	11.327	17.011	1.00	31.82
	1741	N	ASP	A	231		-4.924	11.343	18.246	1.00	30.72
	1742	CA	ASP	A	231		-5.245	12.752	18.060	1.00	32.63
	1743	CB	ASP	A	231		-6.742	12.955	18.305	1.00	35.43
	1744	CG	ASP	A	231		-7.201	12.362	19.639	1.00	41.36
30	1745	OD1	ASP	A	231		-8.426	12.353	19.910	1.00	51.61
	1746	OD2	ASP	A	231		-6.333	11.905	20.422	1.00	31.99
	1747	С	ASP	A	231		-4.443	13.634	19.011	1.00	36.99
	1748	0	ASP	A	231		-3.603	13.145	19.766	1.00	37.67
	1749	N	GLU	A	232		-4.709	14.938	18.960	1.00	40.17
35	1750	CA	GLU	Α	232		-4.033	15.898	19.822	1.00	36.69
	1751	CB	GLU	A	232		-4.459	17.325	19.459	1.00	27.12
	1752	CG	GLU	A	232		-3.880	18.399	20.370	1.00	35.46
	1753	CD	GLU	A	232		-4.364	19.805	20.039	1.00	35.04
	1754	OE1	GLU	A	232		-5.581	20.066	20.113	1.00	37.13
40	1755	OE2	GLU	A	232		-3.525	20.662	19.709	1.00	31.43
	1756	С	GLU	Α	232		-4.389	15.595	21.275	1.00	35.17
	1757	0	GLU	A	232	*	-3.542	15.670	22.160	1.00	34.55
	1758	N	ALA	A	233		-5.646	15.237	21.514	1.00	34.03

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	1803	CG1	l ILE A	239		2.547	15.698	26.093	1.00	16.92
	1804	CDI	l ILE A	239		2.717	16.967	25.299	1.00	28.23
	1805	С	ILE A	239		1.446	14.889	29.640	1.00	30.58
5	1806	0	ILE A	239		2.272	15.270	30,462	1.00	27.47
	1807	N	LEÚ A	240		0.165	14.745	29.934	1.00	30.48
	1808	CA	LEU A	240		-0.290	14.977	31.291	1.00	34.89
	1809	СВ	LEU A	240		-1.816	14.989	31.356	1.00	48.13
	1810	CG	LEU A	240		-2.523	16.290	30.988	1.00	43.96
10	1811	CD1	LEU A	240		-4.015	16.091	31.098	1.00	40.59
	1812	CD2	LEU A	240		-2.077	17.399	31.918	1.00	43.57
	1813	С	LEU A	240		0.254	13.849	32.163	1.00	31.63
	1814	0	LEU A	240	•	0.977	14:086	33.130	1.00	33.47
	1815	N	ALA A	241		-0.088	12.618	31.800	1.00	33.00
15	1816	CA	ALA A	241		0.353	11.440	32.536	1.00	35.65
	1817	CB	ALA A	241		-0.309	10.188	31.965	1.00	36.36
	1818	С	ALA A	241		1.860	11.284	32.493	1.00	40.07
	1819	0	ALA A	241		2.374	10.215	32.789	1.00	43.62
	1820	N	TYR A	242		2.565	12.347	32.128	1.00	46.16
20	1821	CA	TYR A	242		4.018	12.297	32.036	1.00	49.44
	1822	CB	TYR A	242		4.550	13.607	31.461	1.00	42.71
	1823	CG	TYR A	242		6.049	13.671	31.333	1.00	37.89
	1824	CD1	TYR A	242		6.790	12.555	30.962	1.00	38.49
	1825	CE1	TYR A	242		8.173	12.630	30:821	1.00	37.07
25	1826	CD2	TYR A	242		6.724	14.863	31.557	1.00	33.74
	1827	CE2	TYR A	242	. ,	8.096	14.953	31.416	1.00	31.74
	1828	CZ	TYR A	242		8.817	13.840	31.050	1.00	33.16
	1829	ОН	TYR A	242		10.181	13.954	30.909	1.00	32.83
	1830	С	TYR A	242		4.668	11.989	33.378	1.00	56.18
30	1831	0	TYR A	242		4.608	10.847	33.840	1.00	77.34
	1832	N _.	ASN A	243		5.294	12.978	34.010	1.00	62.00
	1833	CA	ASN A	243		5.936	12.715	35.296	1.00	65.83
	1834	CB	ASN A				13.836		1.00	65.24
25	1835	CG	ASN A			8.271	13.304	36.118	1.00	65.31
35	1836		ASN A			8.971	12.630	35.366	1.00	63.84
	1837		ASN A			8.643	13.607	37.354	1.00	65.91
	1838	С	ASN A			4.857	12.567	36.367	1.00	69.21
•	1839		ASN A			3.934	13.388	36.456	1.00	69.74
40	1840	N	ARG A			4.971	11.499	37.159	1.00	68.62
40	1841	CA	ARG A			4.010	11.193	38.221	1.00	71.05
	1842	СВ	ARG A			2.782	10.491	37.626	1.00	71.10
	1843		ARG A				10.186	38.633	1.00	72.04
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	87	С	ILE		25		14.239	-6.516	38.179	1.00 34.24
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	90	CA	ILE	В	26		13.955	-4.132	38.666	
	91	СВ	ILE	В	26		13.754	-2.969	37.661	1.00 32.81
	92	CG2	ILE	В	26		14.178	-1.662	38.291	1.00 24.54
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	96	O .	ILE	В	26		11.920	-3.434	39.757	1.00 33.26
	97	N	MET	В	27		13.553	-4.285	41.064	1.00 39.29
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	101	SD	MET	В	27		15.109	-7.089	43.851	1.00 28.20
	102	CE	MET		. 27		16.507	-7.243	42.803	1.00 29.62
0.5	103	C	MET	В	27		12.687	-2.787	42.884	1.00 41.49
25	104	0	MET	В	27		13.707	-2.156	43.172	1.00 44.33
	105	N	ASP		28		11.448	-2.333	43.057	1.00 38.82
	106	CA	ASP		28		11.135	-1.030	43.624	1.00 37.15
	107	CB	ASP.		28		10.613	-0.088	42.536	1.00 36.09
30	108	CG	ASP		28		11.704	0.755	41.931	1.00 37.61
30	109	OD1			28		12.621		41.305	1.00 40.92
	110		ASP		28		11.646		42.091	
	111	C	ASP		28		10.071	-1.183		1.00 37.00
	112 113	0 N	ASP		28		9.342	-2.176	44.716	
35	114	N CA	GLY		29		9.989	-0.198	45.584	1.00 32.98
55	115	CA	GLY		29		8.997	-0.237	46.639	1.00 31.71
	116	0	GLY		29		9.576	-0.501	48.012	1.00 34.52
	117	N	GLY		29		8.905	-0.295	49.015	1.00 35.45
	118	CA	ASN		30		10.822	-0.959	48.061	1.00 35.21
40	119	CB	ASN ASN		30 30		11.479	-1.259	49.322	1.00 34.55
. •	120	CG	ASN :		30		12.982	-1.388	49.101	1.00 21.98
	121		ASN :				13.372	-2.739 -2.070	48.528	1.00 23.62
	122		ASN :		30		14.537		48.222	1.00 20.30
		1102	HOM .	ت	30		12.397	-3.634	48.392	1.00 20.74

	123	С	ASN	1 в	30	11.195	-0.224	50.395	1.00 38.93
	124	0	ASN	1 B	30	10.527	-0.521	51.381	1.00 42.50
	125	N	GLY	B	31	11.693	0.992	50.199	1.00 38.13
	126	CA	GL)	? В	31	11.481	2.053	51.173	1.00 37.44
5	127	С	GL	. В	31	10.033	2.484	51.353	1.00 37.86
	128	0	GLY	' В	31	9.592	2.784	52.460	1.00 33.07
	129	N	ARG	В	32	9.291	2.532	50.256	1.00 41.86
	130	CA	ARG	В	32	7.890	2.920	50.300	1.00 43.79
	131	CB	ARG	B	32	7.331	2.969	48.876	1.00 50.98
10	132	CG	ARG	; в	32	5.999	3.679	48.722	1.00 67.82
	133	CD	ARG	В	32	5.606	3.727	47.254	1.00 72.94
	134	NE	ARG	В	32	4.186	4.006	47.062	1.00 79.64
	135	CZ	ARG	В	32	3.538	3.824	45.914	1.00 90.52
	136	NHl	ARG	В	32	4.186	3.365	44.849	1.00100.13
15	137	NH2	ARG	В	32	2.241	4.091	45.830	1.00 94.94
	138	С	ARG	В	32	7.171	1.867	51.135	1.00 41.07
	139	0	ARG	В	32	6.348	2.194	51.983	1.00 39.65
	140	N	TRP	В	33	7.510	0.605	50.885	1.00 39.29
,	141	CA	TRP	В	33	6.948	-0.546	51.593	1.00 37.27
20	142	CB	TRP	В	33	7.593	-1.834	51.081	1.00 28.51
	143	CG	TRP	В	33	7.184	-3.076	51.818	1.00 29.95
	144	CD2	TRP	В	33	7.882	-3.701	52.900	1.00 34.19
	145	CE2	TRP	В	33	7.137	-4.836	53.277	1.00 29.68
	146	CE3	TRP	В	33	9.065	-3.407	53.590	1.00 47.07
25	147	CD1	TRP	В	33	6.076	-3.835	51.592	1,00 35.81
•	148	NE1	TRP	В	33	6.040	-4.896	52.462	1.00 31.40
	149	CZ2	TRP	В	33	7.536	-5.684	54.316	1.00 27.96
	150	CZ3	TRP	В	33	9.460	-4.251	54.624	1.00 47.40
	151	CH2	TRP	В	33	8.696	-5.375	54.976	1.00 33.44
30	152	С	TRP	В	33	7.230	-0.428	53.085	1.00 35.31
	153	0	TRP	В	33	6.345	-0.603	53.918	1.00 35.16
	154	N	ALA	В	34	8.485	-0.151	53.408	1.00 30.64
	155	CA	ALA	В	34	8.907	-0.006	54.791	1.00 26.94
	156	CB	ALA		34	10.420	0.130	54.849	1.00 21.71
35	157	С	ALA	В	34	8.249	1.214	55.431	1.00 29.54
	158	0	ALA	В	34	7.619	1.118	56.487	1.00 30.57
	159	N	LYS	В	35	8.397	2.359	54.773	1.00 30.23
	160	CA	LYS	В	35	7.851	3.612	55.263	1.00 32.86
	161	CB	LYS	В	35	8.129	4.725	54.249	1.00 42.27
40	162	CG	LYS		35	8.577	6.048	54.859	1.00 58.11
	163	CD	LYS	В	35	8.488	7.167	53.834	1.00 74.59
	164	CE	LYS	В	35	7.059	7.302	53.311	1.00 85.25
	165	NZ	LYS	В	35	6.928	8.270	52.191	1.00 84.42

	166	С	LY:	s B	35		6.353	3.523	55.551	1.00	38.17
	167	0	LY:	з в	35		5.835	4.257	56.390	1.00	41.62
	168	N	LYS	з в	36		5.652	2.624	54.870	1.00	41.65
	169	CA	LYS	S B	36		4.219	2.498	55.094	1.00	43.49
5	170	СВ	LYS	з в	36		3.519	1.935	53.850	1.00	52.09
	171	CG.	LYS	з в	36		3.680	0.428	53.648	1.00	61.96
	172	CD	LYS	з в	36		2.834	-0.098	52.468	1.00	65.82
	173	CE	LYS	з в	36		2.974	-1.623	52.289	1.00	62.88
	174	NZ	LYS	3 B	36		2.084	-2.191	51.225	1.00	66.92
10	175	С	LYS	з в	36		3.926	1.613	56.300	1.00	44.16
	176	0	LYS	3 B	36		2.857	1.706	56.895	1.00	46.34
	177	N	ARC	3 B	37		4.877	0.762	56.668	1.00	44.81
	178	CA	ARC	3 B	37		4.691	-0.129	57.803	1.00	46.91
	179	CB	ARC	3 B	37		5.305	-1.498	57.521	1.00	54.16
15	180	CG	ARC	3 B	37		4.652	-2.223	56.372	1.00	51.20
	181	CD	ARG	В	37		5.258	-3.588	56.141	1.00	52.57
	18,2	NE	ARG	; B	37		4.915	-4.074	54.808	1.00	61.49
	183	CZ	ARG	; B	37		3.675	-4.307	54.387	1.00	65.32
	184	NH1	ARG	В	37		2.653	-4.107	55.206	1.00	68.41
20	185	NH2	ARG	В	37		3.454	-4.713	53.140	1.00	59.01
	186	С	ARG	В	37		5.280	0.418	59.087	1.00	46.38
	187	0	ARG	В	37		5.519	-0.331	60.024	1.00	45.99
	. 188	N	MET	В	38		5.526	1.721	59.135	1.00	46.89
	189	CA	MET	В	38		6.069	2.346	60.338	1.00	49.02
25	190	CB	MET	В	38		5.216	1.987	61.564	1.00	46.95
	191	CG	MET	В	38		3.709	2.133	61.400	1.00	54.51
	192	SD	MET	В	38		3.148	3.835	61.214	1.00	62.23
	193	CE	MET	В	38		3.372	4.473	62.901	1.00	68.23
20	194	С	MET		38		7.517	1.960	60.652	1.00	49.28
30	195	0	MET		38		8.062		61.662	1.00	50.06
	196	N	GLN				8.148		59.821	1.00	49.00
	197	CA	GLN		39		9.521	0.750	60.118	1.00	48.43
	198	CB	GLN		39		9.673		60.007	1.00	40.73
25	199	CG	GLN		39			-1.431	58.920		51.03
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	201		GLN			•	9.897	-3.586	59.055		57.42
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	203	С	GLN		39		10.589	1.455	59.298	1.00	50.38
40	204	0	GLN		39		10.310	2.002	58.239	1.00	52.17
40	205	N	PRO		40		11.837	1.455	59.792		51.48
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	207	CA	PRO		40	٠	12.958	2.100	59.108	1.00	49.78
	208	СВ	PRO	В	40		14.174	1.500	59.810	1.00	50.09

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5	256	CA	LYS	3.B	46		16.018	-6.734	53.821	1.00	36.56
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	258	CG	LYS	В	46	•	16.277	-8.288	55.800	1.00	36.67
	259	CD	LYS	В	46		16.525	-8.385	57.301	1.00	47.11
	260	CE	LYS	В	46	•	17.756	-7.581	57.721	1.00	45.30
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	263	0	LYS	В	46		14.970	-8.572	52.714	1.00	34.48
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	265	CA	ALA	В	47		12.404	-7.552	53.019	1.00	33.65
15	266	CB	ALA	В	47	•	11.205	-6.669	53.346	,1.00	22.25
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	269	N	GLY	В	48		13.048	-6.812	50.787	1.00	31.73
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20	271	С	GLY	В	48		13.881	-8.307	49.194	1.00	28.17
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	273	N	MET	В	49		15.027	-8.448	49.848	1.00	26.41
	274	CA	MET	В	49	• .	15.801	-9.677	49.787	1.00	26.13
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25	276	CG	MET	В	49		17.778	-10.911	50.907	1.00	31.14
	277	SD	MET.	·B	49		19.315	-10.778	51.891	1.00	30.86
	278	CE	MET	В	49		18.675	-10.085	53.433	1.00	27.72
	279	С	MET	В	49		14.951	-10.894	50.128	1.00	26.86
	280	0	MET	В	49		15.075	-11.936	49.493	1.00	25.74
30	281	N	GLU	В	50		14.087	-10.773	51.128	1.00	26.86
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	284	CG	GLU		50		13.166	-11.100	53.881	1.00	42.20
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35	286		GLU		50		12.645	-13.028	55.166	1.00	54.70
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	288	С	GLU	В	50		12.380	-12.318	50.308	1.00	33.72
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	363	CG	LYS		61	•	7.504	-23.750	41.382	1.00	49.61
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	.365	CE	LYS		61		5.080	-23.562	42.030	1.00	76.26
••	366	ΝZ	LYS		61			-23.993	42.958	1.00	77.30
30	367	С	LYS		61		8.910	-24.362	39.143	1.00	41.26
	368	0	LYS		61			-25.321	38.702		38.34
	369	N	LEU		62		8.894	-23.170	38.570	1.00	43.33
	370	CA	LEU		62			-22.921	37.379		40.43
~ -	371	СВ	LEU		62			-21.541	37.478		41.05
35	372	CG	LEU		62			-21.307	36.709		43.45
	373		LEU		62			-22.374	37.061		49.97
	374		LEU		62			-19.933	37.055		41.95
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40	377	N	GLY		63			-23.404	36.292		34.00
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	379	С	GLY		63			-22.368	34.483		34.70
	380	0	GLY	В	63		12.311	-22.494	33.400	1.00	37.15

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	382	CA	VAL		64			-20.051	34.475		33.85
	383	СВ	VAL		64			-18.780	35.297		38.31
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	386	C	VAL	В	64			-20.376	34.449		32.11
	387	0	VAL	В	64			-20.691	35.478		35.71
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	389	CA	LYS	B	65		15.830	-20.629	33.178	1.00	32.19
10	390	СВ	LYS	В	65		16.276	-20.642	31.720	1.00	34.45
	391	CG	LYS	В	65		16.629	-22.024	31.194	1.00	28.19
	392	CD	LYS	В	65		15.416	-22.950	31.165	1.00	32.70
	393	CE	LYS	В	65		15.722	-24.264	30.438	1.00	50.92
	394	NZ	LYS	В	65		16.090	-24.081	28.994	1.00	60.18
15	395	С	LYS	В	65		16.738	-19.695	33.963	1.00	32.24
	396	0	LYS	В	65		17.634	-20.152	34.667	1.00	32.31
	397	N	VAL	В	66		16.515	-18.389	33.843	1.00	29.19
	398	CA	·VAL	В	66		17.342	-17.402	34.547	1.00	27.66
	399	СВ	VAL	В	66		18.647	-17.103	33.727	1.00	30.38
20	400	CG1	VAL	В	66		18.369	-17.285	32.254	1.00	29.01
	401	CG2	VAL	В	66		19.170	-15.681	34.002	1.00	16.92
	402	С	VAL	В	66		16.623	-16.087	34.846	1.00	22.57
	403	0	VAL	В	66		15.637	-15.758	34.199	1.00	18.50
	404	N	ILE	В	67		17.099	-15.360	35.855	1.00	23.89
25	405	CA	ILE	В	67		16.533	-14.054	36.196	1.00	31.24
٠.	406	CB	ILE	В	67		15.389	-14.129	37.259	1.00	30.49
	407	CG2	ILE	В	67		14.278	-15.044	36.761	1.00	32.00
	408	CG1	ILE	В	67		15.920	-14.612	38.604	1.00	35.49
20	409		ILE		67			-14.690	39.664	1.00	44.48
30	410	С	ILE		67			-13.112	36.685	1.00	32.32
	411	0	ILE		67		18.497	-13.490	37.483	1.00	36.35
	412	N	THR		68			-11.890	36.160	1.00	27.06
	413	CA	THR		68			-10.854	36.497	1.00	22.58
25	414	СВ	THR		68			-10.256	35.239		20.26
35	415		THR		68			-11.283	34.524	1.00	31.06
	416		THR					-9.135	35.606	1.00	16.92
	417	С	THR		68		17.854	-9.756	37.281	1.00	26.08
	418	0	THR		68		17.017	-9.027	36.751	1.00	28.24
40	419	N	VAL		69		18.210	-9.663	38.557	1.00	25.72
40	420		VAL		69		17.631		39.475		22.44
	421	CB	VAL		69		17.459	-9.329	40.845		20.89
	422		VAL		69			-10.430	40.788	1.00	16.92
	423	CG2	VAL	В	69		18.784	-9.901	41.301	1.00	16.92

	424	С	VAL	В	69	18.536	-7.495	39.614	1.00 23.00
	425	0	VAL	В	69	19.720	-7.635	39.923	1.00 23.85
	426	N	TYR	В	70	17.977	-6.313	39.375	1.00 25.89
	427	CA	TYR	В.	70	18.732	-5.066	39.489	1.00 26.71
5	428	CB	TYR	В	70	17.978	-3.926	38.798	1.00 22.08
	429	CG-	TYR	В	70	18.861	-2.795	38.312	1.00 16.92
	430	CD1	TYR	В	70	20.240	-2.807	38.539	1.00 16.92
	431	CE1	TYR	В	70	21.056	-1.781	38.067	1.00 16.92
	432	CD2	TYR	В	70	18.320	-1.720	37.597	1.00 18.76
. 10	433	CE2	TYR	В	70	19.125	-0.689	37.121	1.00 20.19
	434	CZ	TYR	В	70	20.490	-0.728	37.359	1.00 23.85
	435	ОН	TYR	В	70	21.290	0.283	36.889	1.00 28.88
	436	С	TYR	В	70	18.895	-4.756	40.981	1.00 27.42
	437	0	TYR	В	70	18.045	-4.077	41.579	1.00 29.24
15	438	N	АĻА	В	71	19.991	-5.258	41.560	1.00 26.20
	439	CA	ALA	В	71	20.303	-5.103	42.984	1.00 27.77
	440	CB	ALA	В	71	21.123	-6.301	43.448	1.00 21.40
	441	С	ALA	В	71	20.996	-3.798	43.418	1.00 33.28
	442	0	ALA	В	71	20.758	-3.301	44.519	1.00 35.06
20	443	N	PHE	В	72	21.867	-3.247	42.580	1.00 34.13
	444	CA	PHE	В	72	22.533	-1.999	42.938	1.00 35.25
	445	СВ	PHE	В	72	23.672	-2.263	43.937	1.00 28.54
	446	CG	PHE	В	72	24.179	-1.017	44.624	1.00 32.61
	447	CD1	PHE	В	72	23.480	-0.458	45.694	1.00 33.56
25 .	448	CD2	PHE	В	72	25.332	-0.374	44.179	1.00 35.80
	449	CE1	PHE	В	72	23.924	0.726	46.309	1.00 28.42
	450	CE2	PHE	В	72	25.777	0.807	44.788	1.00 32.48
	451	CZ	PHE	В	72	25.070	1.355	45.854	1.00 31.11
	452	С	PHE	В	72	23.079	-1.313	41.689	1.00 40.63
30	453	0	PHE	В	72	24.052	-1.770	41.102	1.00 43.32
	454	N	SER	В	73	22.447	-0.217	41.279	1.00 47.02
	455	CA	SER	В	73	22.893	0.514	40.093	1.00 49.68
	456	СВ	SER	В	73	21.794	1.441	39.575	1.00 43.74
	457	OG	SER	В	73	21.824	2.681	40.257	1.00 33.26
35	458	С	SER	В	73	24.119	1.351	40.423	1.00 52.36
	459	0	SER	В	73	24.433	1.577	41.593	1.00 53.00
	460	N	THR	В	74	24.804	1.816	39.386	1.00 57.20
	461	CA	THR	В	74	25.996	2.630	39.573	1.00 62.04
	462	CB	THR	В	74	26.707	2.904	38.214	1.00 67.14
40	463	OG1	THR	В	74	26.682	1.723	37.404	1.00 74.37
	464	CG2	THR	В.	74	28.159	3.292	38.440	1.00 71.77
	465	С	THR	В	74	25.569	3.956	40.199	1.00 62.95
	466	0	THR	В	74	26.316	4.582	40.951	1.00 62.39

	467	N	GLU	В	75	24.340	4.360	39.900	1.00 63.63
	468	CA	GLU	В	75	23.804	5.621	40.394	1.00 66.15
	469	СВ	GLU	В	75	22.783	6.165	39.389	1.00 75.90
	470	CG	GLU	В	75	22.350	7.593	39.651	1.00 93.53
5	471	CD	GLU	В	75	21.286	8.057	38.686	1.00103.81
	472	OE1	GLU	· B	75	20.236	7.384	38.593	1.00110.70
	473	OE2	GLU	В	75	21.500	9.094	38.023	1.00111.36
	474	С	GLU	В	75	23.168	5.533	41.779	1.00 66.40
	475	0	GLU	В	75	22.464	6.450	42.203	1.00 68.91
10	476	N	ASN	В	76	23.415	4.439	42.490	1.00 64.57
	477	CA	ASN	₿	76·	22.845	4.281	43.825	1.00 59.63
	478	СВ	ASN	В	76	22.419	2.827	44.067	1.00 53.70
	479	CG	ASN	В	76	21.031	2.531	43.539	1.00 46.89
	480	OD1	ASN	В	76	20.101	3.305	43.752	1.00 50.66
15	481	ND2	ASN	В	76	20.880	1.402	42.861	1.00 40.20
	482	С	ASN	В	76	23.774	4.727	44.950	1.00 56.27
	483	0	ASN	В	76	23.319	4.953	46.071	1.00 55.41
	484	N	TRP	В	77	25.067	4.860	44.657	1.00 53.67
	485	CA	TRP	В	77	26.026	5.270	45.679	1.00 51.94
20	486	СВ	TRP	В	77	27.460	5.237	45.132	1.00 48.90
	487	CG	TRP	В	77	27.920	3.896	44.617	1.00 51.60
	488	CD2	TRP	В	77. ·	28.576	2.859	45.365	1.00 51.70
	489	CE2	TRP	В	77	28.839	1.797	44.467	1.00 52.11
	490	ÇE3	TRP	В	77 , 2,	28.968	2.722	46.706	1.00 43.86
25	491	CD1	TRP	В	77	27.812	3.431	43.338	1.00 52.12
	492	NE1	TRP	В	77	28.362	2.173	43.240	1.00 53.74
	493	CZ2	TRP	В	77	29.476	0.616	44.865	1.00 43.91
	494	CZ3	TRP	В	77	29.603	1.540	47.101	1.00 37.41
	495	CH2	TRP	В	77	29.850	0.506	46.180	1.00 35.61
30	496	С	TRP	В	77	25.701	6.676	46.181	1.00 50.29
	497	0	TRP	В	77	26.194	7.112	47.226	1.00 54.30
	498	N	THR	В	78	24.858	7.369	45.428	1.00 46.30
	499	CA	THR	В	78	24.434	8.726	45.751	1.00 40.87
	500	СВ	THR		78	23.518	9.268	44.646	1.00 40.94
35	501		THR		78	24.257	9.344	43.421	1.00 41.23
	502		THR		78	22.972	10.641	45.013	1.00 43.72
	503	С	THR	В	78	23.685	8.805	47.076	1.00 39.63
	504	0	THR	В	78	23.558	9.881	47.661	1.00 43.77
40	505	N	ARG		79	23.194		47.548	1.00 33.93
40	506	CA	ARG		79	22.424	7.593	48.792	1.00 29.09
	507	СВ	ARG		79	21.698		48.855	1.00 22.71
	508	CG	ARG		79	20.705		47.730	1.00 24.31
	509	CD	ARG	В	79	20.027	4.767	47.718	1.00 23.41

	510	NE	ARG	B	79		18.813	4.835	46.916	1.00	19.61
	511	CZ	ARG	В	79		17.945	3.839	46.780	1.00	25.88
	512	NH1	. ARG	; в	79		18.159	2.683	47.396	1.00	35.60
	513	NH2	ARG	'B	79	•	16.858	4.004	46.037	1.00	23.97
5	514	С	ARG	. B	79		23.217	7.830	50.076	1.00	31.63
	515	0	ARG	В	79	٠.	24.447	7.732	50.094	1.00	31.85
	516	N	PRC	В	80		22.513	8.167	51.171	1.00	30.10
	517	CD	PRC	В	80		21.059	8.319	51.358	1.00	30.04
	518	CA	PRO	В	80	•	23.233	8.402	52.423	1.00	31.57
10	519	СВ	PRO	В	80,		22.113	8.754	53.414	1.00	29.71
	520	CG	PRO	В	80		20.904	8.083	52.840	1.00	29.28
	521	С	PRO	В	80	•	24.041	7.168	52.824	1.00	38.32
	522	0	PRO	В	80		23.487	6.083	53.011	1.00	42.42
	523	N	ASP	В	81		25.356	7.351	52.935	1.00	4,1.93
15	524	CA	ASP	В	81	•	26.284	6.284	53.299	1.00	45.58
	525	CB	ASP	В	81		27.427	6.850	54.150	1.00	63.07
	526	CG	ASP	В	81		28.116	8.043	53.504	1.00	67.38
	527	OD1	ASP	В	81		28.509	7.948	52.321	100	73.52
	528	OD2	ASP	В	81		28.274	9.075	54.189	1.00	72.51
,20	529	С	ASP	В	81		25.616	5.136	54.055	1.00	44.34
	530	0	ASP	В	81		25.671	3.984	53.626	1.00	45.14
	531	N	GLN	В	82		24,981	5.456	55.178	1.00	43.19
	532	CA	GLN	В	82		24.316	4.443	55.981	1.00	46.00
	533	CB	GLN	В	82		23.492	5.110	57.076	1.00	45.03
25	534	CG	GLN	В	82		24.289	5.374	58.335	1.00	34.60
	535	CD	GLN		82		24.607	4.099	59.104	1.00	16.92
	536		GLN		82		23.720	3.476	59.693	1.00	26.54
	537	NE2			82		25.875	3.703	59.098	1.00	16.92
••	538	С	GLN		82		23.448	3.473	55.187	1.00	47.51
30	539	0	GLN		82		23.598	2.260	55.322	1.00	51.03
	540	N	GLU		83		22.541	3.998	54.367	1.00	44.67
	541	CA	GLU		83		21.667	3.142	53.565	1.00	37.68
	542	CB	GLU		83		20.754	3.979	52.664		35.83
25	543	CG	GLU		83		19.621	3.191	52.003	1.00	39.43
35	544	CD	GLU		83		18.718	4.065	51.137		43.90
	545		GLU		83		17.556	3.666	50.877	1.00	48.19
	546		GLU		83		19.176	5.149	50.706	1.00	48.89
	547	С	GLU		83		22.517	2.232	52.700	1.00	32.89
40	548		GLU		83		22.222	1.054	52.566	1.00	32.08
40	549	N	VAL		84		23.571	2.787	52.109	1.00	30.13
	550		VAL		84		24.464	1.998	51.273	1.00	31.93
	551	СВ	VAL		84		25.503	2.884	50.546	1.00	35.84
	552	CG1	VAL	В	84		26.379	2.025	49.640	1.00	39.26

	553	CG2	VAI	ъВ	84		24.792	3.946	49.722	1.00	34.99	
	554	·C	VAI	ъВ	84		25.177	1.016	52.196	1.00	33.63	
	555	0	VAI	ъВ	84		25.276	-0.178	51.903	1.00	34.73	
	556	N	LYS	в в	85		25.667	1.533	53.319	1.00	33.74	
5	557	CA	LYS	B	85		26.341	0.716	54.322	1.00	35.59	
	558	СВ	LYS	В	85		26.496	1.544	55.612	1.00	48.55	
	559	CG	LYS	В	85		26.571	0.767	56.928	1.00	59.03	
	560	CD	LYS	В	85		27.942	0.170	57.196	1.00	67.33	
	561	CE	LYS	B	85		27.943	-0.586	58.525	1.00	72.93	
10	562	NZ	LYS	В	85		29.237	-1.290	58.785	1.00	68.29	
,	563	С	LYS	В	85		25.464	-0.525	54.545	1.00	33.73	
	564	0	LYS	В	85		25.918	-1.655	54.380	1.00	32.87	
	565	N	PHE	В	86	,	24.200	-0.280	54.882	1.00	34.91	
	566	CA	PHE	В	86		23.192	-1.314	55.132	1.00	38.00	
15	567	CB	PHE	В	86		21.840	-0.640	55.405	1.00	29.90	
	568	CG	PHE	В	86		20.701	-1.600	55.644	1.00	28.19	
	569	CD1	PHE	В	86		20.164	-1.758	56.918	1.00	28.34	
	570	CD2	PHE	В	86		20.112	-2.289	54.586	1.00	30.14	
	571	CE1	PHE	В	86		19.052	-2.581	57.133	1.00	16.92	
20	572	CE2	PHE	В	86		19.004	-3.114	54.792	1.00	31.79	
	573	CZ	PHE	В	86		18.472	-3.258	56.067	1.00	23.42	
	574	С	PHE	В	86		23.039	-2.310	53.982	1.00	41.33	
	575	0	PHE	В	86		23.232	-3.512	54.170	1.00	44.39	
	576	N	ILE	В	87		22.674	-1.811	52.800	1.00	42.94	
25	577	CA	ILE	В	87		22.479	-2.661	51.624	1.00	44.91	
	578	CB	ILE	В	87		22.225	-1.831	50.348	1.00	33.27	
	579	CG2	ILE		87		21.956	-2.748	49.176	1.00	35.47	
	580	CG1	ILE		87		21.018	-0.925	50.538	1.00	33.55	
20	581	CD1	ILE		87		20.762	-0.027	49.357	1.00	34.35	
30	582	С	ILE		87		23.683	-3.552	51.354		49.45	
	583	0	ILE		87		23.559		51.312		51.81	
	584	N ~-	MET		88		24.845	-2.933	51.174		49.47	
	585	CA	MET		88		26.064	-3.680	50.892		49.30	
35	586	CB	MET		88		27.269	-2.737	50.822		50.22	
رد	587	CG	MET		88			-1.661			45.64	
	588	SD	MET				26.855	-2.262	48.067		36.68	
	589	CE	MET		88		28.205	-3.366	47.823		32.68	
	590	C	MET		88		26.352	-4.815	51.881		47.36	
40	591	0	MET		88			-5.678	51.614		47.71	
+0	592	N	ASN		89		25.676	-4.835	53.022		47.87	
	593	CA	ASN		89			-5.919	53.958		53.55	
	594 505	CB	ASN		89			-5.421	55.400		59.69	
	595	CG	ASN	В	89		26.446	-6.481	56.358	1.00	60.29	

	596	OD1	ASN	В	89		27.611	-6.880	56.300	1.00	58.66
	597	ND2	ASN	В	89		25.567	-6.956	57.233	1.00	59.82
	598	С	ASN	В	89		24.874	-7.011	53.814	1.00	54.69
	599	0	ASN	В	89		24.876	-7.996	54.555	1.00	55.77
5	600	N	LEU	В	90		23.971	-6.821	52.856	1.00	53.91
	601	CA	LEU	В	90		22.919	-7.792	52.593	1.00	50.26
	602	СВ	LEU	В	90		21.804	-7.158	51.759	1.00	44.32
	603	CG	LEU	В	90		20.892	-6.161	52.478	1.00	38.54
	604	CD1	LEU	В	90		19.928	-5.544	51.488	1.00	43.04
. 10	605	CD2	LEU	В	90		20.129	-6.869	53.578	1.00	42.59
	606	С	LEU	В	90		23.492	-9.013	51.879	1.00	47.14
	607	0	LEU	В	90		22.974	-10.121	52.027	1.00	44.55
	608	N	PRO	В	91		24.556	-8.825	51.072	1.00	46.27
	609	CD	PRO	В	91		25.020	-7.553	50.489	1.00	44.80
15	610	CA	PRO	В	91		25.162	-9.958	50.366	1.00	46.47
	611	CB	PRO	В	91		26.199	-9.285	49.470	1.00	43.34
	612	CG	PRO	В	91		25.545	-7.993	49.145	1.00	45.54
	613	С	PRO	В	91		25.795	-10.958	51.346	1.00	47.41
	614	0	PRO	В	91		26.062	-12.107	51.000	1.00	46.38
20	615	N	VAL	В	92		26.033	-10.507	52.573	1.00	47.94
	616	CA	VAL	В	92		26.619	-11.363	53.598	1.00	45.52
	617	CB	VAL	В	92		27.367	-10.537	54.639	1.00	34.17
	618	CG1	VAL	В	92		28.018	-11.454	55.632	1.00	38.02
	619	CG2	VAL	В	92		28.404	-9.666	53.957	1.00	38.64
25.	620	С	VAL	В	92		25.512	-12.154	54.286	1.00	45.50
	621	0	VAL	В	92		25.576	-13.379	54.364	1.00	44.68
	622	N	GLU	В	93		24.499	-11.447	54.782	1.00	42.90
	623	CA	GLU	В	93		23.367	-12.099	55.418	1.00	42.53
	624	CB	GLU	В	93		22.252	-11.101	55.707	1.00	49.87
30	625	CG	GLU	В	93		22.684	-9.832	56.407	1.00	57.60
	626	CD	GLU		93	•	21.498	-9.061	56.963	1.00	61.78
	627		GLU		93		21.693	-7.934	57.473	1.00	71.50
	628	OE2	GLU	В	93		20.367	-9.592	56.892	1.00	52.19
	629	С	GLU	В	93		22.844	-13.111	54.412	1.00	43.12
35	630	0	GLU		93		22.582	-14.263	54.742	1.00	45.85
	631	N	PHE		94		22.694	-12.661	53.172	1.00	45.41
	632	CA	PHE		94			-13.515	52.101	1.00	46.26
	633	СВ	PHE		94		22.269	-12.780	50.761	1.00	42.53
46	634	CG	PHE		94			-13.507	49.645	1.00	32.85
40	635		PHE		94			-13.595	49.617	1.00	28.47
	636		PHE		94			-14.148	48.649	1.00	28.12
	637		PHE		94		19.523	-14.314	48.617	1.00	19.92
	638	CE2	PHE	В	94		21.666	-14.870	47.644	1.00	31.07

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639
           CZ
               PHE B
                       94
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	773	OE1	L GLN	E	110	٠.	25.989	-18.516	35.741	1.00	42.83
	774	NE2	GLN	E	110		26.363	-16.329	35.331	1.00	66.31
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	776	0	GLN	B	110	٠	24.671	-13.423	39.890	1.00	36.09
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	788				112			-10.321			34.53
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	809		THR				33.791	-7.038	40.891	1.00	
•	810		THR				31.409	-7.332 -7.500	40.244		53.59
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	818	OD2	ASP	В	116	38.262	-4.723	39.860	1.00 75.26
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	829	NH2	ARG	В	117	33.381	1.264	37.300	1.00131.90
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,	834	CB	LEU	В	118	31.834	-4.402	45.573	1.00 53.32
25	835	CG	LEU	В	118	30.831	-4.440	44.427	1.00 51.22
	836	CD1	LEU			30.449	-5.893	44.140	1.00 43.14
	837	CD2				29.599	-3.618	44.800	1.00 48.18
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	843	CB	PRO			32.010			
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                              26.199 -2.844
                                              41.316 1.00 36.56
     1052
           CA
               ASN B 146
                              27.025 -1.741
                                              40.844
                                                      1.00 38.10
     1053
               ASN B 146
           CB
                              28.443
                                      -1.818
                                              41.416
                                                      1.00 32.16
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               ASN B 146
           CG
                              29.242 -0.554
                                              41.142
                                                      1.00 36.02
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           OD1 ASN B 146
                              28.739
                                      0.556
                                              41.316 1.00 38.28
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           С
               ASN B 146
                              27.051
                                      -1.822
                                              39.318
                                                      1.00 39.84
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           0
               ASN B 146
                              28.062
                                      -1.538
                                              38.675
                                                      1.00 40.22
     1059
           N
               TYR B 147
                              25.907
                                      -2.213
                                              38.758
                                                      1.00 37.99
35
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           CA
               TYR B 147
                              25.720
                                      -2.366
                                              37.320
                                                      1.00 38.54
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           CB
               TYR B 147
                              24.882 -3.615
                                              37.029
                                                      1.00 36.21
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           CG
               TYR B 147
                              24.382
                                      -3.697
                                              35.600
                                                      1.00 32.62
     1063
           CD1 TYR B 147
                              25.147
                                      -4.299
                                              34.602
                                                      1.00 29.51
     1064
           CE1 TYR B 147
                              24.712 -4.318
                                              33.273
                                                      1.00 33.34
40
     1065
           CD2 TYR B 147
                              23.163
                                      -3.118
                                              35.233 1.00 32.87
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           CE2 TYR B 147
                              22.721 -3.130
                                              33.908
                                                      1.00 33.52
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           CZ
               TYR B 147
                              23.499
                                      -3.731
                                              32.934
                                                      1.00 36.75
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          OH TYR B 147
                              23.067
                                      -3.741
                                              31.625
                                                     1.00 40.69
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	1069	С	TYR E	3 147	25.025	-1.167	36.694	1.00	38.81
	1070	0	TYR E	147	24.027	-0.668	37.212	1.00	39.53
	1071	N	GLY E	148	25.553	-0.729	35.559	1.00	34.56
	1072	CA	GLY E	148	24.973	0.390	34.849	1.00	35.29
5	1073	C ·	GLY E	148	24.844	0.084	33.367	1.00	36.55
	1074	0	GLY E	148	25.821	-0.266	32.713	1.00	34.11
	1075	N	GLY E	149	23.635	0.216	32.836	1.00	35.88
	1076	CA	GLY E	149	23.406	-0.053	31.428	1.00	35.86
	1077	С	GLY E	149	24.445	0.531	30.489	1.00	33.73
10	1078	0	GLY E	149	25.268	-0.194	29.924	1.00	34.86
	1079	N	ARG E	150	24.411	1.845	30.308	1.00	29.19
	1080	CA	ARG E	150	25.358	2.498	29.418	1.00	28.55
	1081	CB	ARG E	150	25.124	4.009	29.408	1.00	21.40
	1082	CG	ARG E	150	23.737	4.438	28.938	1.00	21.80
15	1083	CD	ARG E	150	23.659	5.946	28.778	1.00	16.92
	1084	NE	ARG E	150	22.302	6.390	28.487	1.00	16.92
	1085	CZ	ARG E	150	21.961	7.656	28.252	1.00	19.59
	1086	NH1	ARG B	150	22.883	8.614	28.269	1.00	23.32
	1087	NH2	ARG B	150	20.692	7.974	28.008	1.00	21.38
20	1088	C	ARG B	150	26.790	2.197	29.847	1.00	30.06
	1089	0	ARG B		27.701	2.105	29.021	1.00	26.00
	1090	N	ALA B	151	26.983	2.043	31.148	1.00	35.94
•	1091	CA	ALA B		28.304	1.745	31.673	1.00	37.38
~~	1092	CB	ALA B	151	. 28.254	, 1.688	33.194	1.00	52.48
25	1093	С	ALA B		28.823	0.419	31.108	1.00	35.17
٠,	1094	0	ALA B		29.959	0.345	30.635		31.19
	1095	N	GLU B		27.990	-0.620	31.161		32.94
	1096	CA	GLU B		28.362	-1.938	30.655		35.48
20	1097	CB	GLU B		27.220	-2.933	30.859		30.00
30	1098	CG	GLU B						
			GLU B			-5.100			22.76
	1100				25.001		30.160		21.18
	1101 1102		GLU B			-6.344			
35			GLU B			-1.900	,		38.76
		N				-2.473			39.19
	1105	CA	ILE B				28.365		39.55
		СВ	ILE B		28.182	-0.420	26.929		•
			ILE B		27.348				32.60
40			ILE B		25.718		24.692		35.83
					24.555		26.425		37.55
	1110		ILE B			-0.452	25.731		34.30 40.62
	1111		ILE B			-0.747			
		•	D	100	20.213	-0./4/	23.129	1.00	37.23

	1112	N	THR B 154	29.747	0.631	27.446	1.00 45.36
	1113	CA	THR B 154	30.953	1.442	27.298	1.00 47.53
	1114	СВ	THR B 154	30.937	2.624	28.270	1.00 36.71
·	1115	OG	1 THR B 154	29.670	3.278	28.194	1.00 34.10
5	1116	CG	2 THR B 154	32.016	3.617	27.910	1.00 31.30
	1117	C.	THR B 154	32.194	0.601	27.567	1.00 51.16
	1118	. 0	THR B 154	33.211	0.732	26.885	1.00 50.52
	1119	N	GLN B 155	32.099	-0.260	28.572	1.00 55.38
	1120	CA	GLN B 155	33.192	-1.143	28.946	1.00 57.33
10	1121	СВ	GLN B 155	32.855	-1.851	30.264	1.00 67.23
	1122	CG	GLN B 155	33.707	-3.068	30.590	1.00 83.16
	1123	CD	GLN B 155	33.045	-4.380	30.180	1.00 90.67
	1124	OE:	l GLN B 155	33.604	-5.461	30.385	1.00 95.55
	1125	NE2	2 GLN B 155	31.849	-4.291	29.603	1.00 94.98
15	1126	С	GLN B 155	33.418	-2.155	27.832	1.00 56.79
	1127	0	GLN B 155	34.555	-2.448	27.470	1.00 57.35
	1128	N	ALA B 156	32.327	-2.680	27.284	1.00 54.82
	1129	CA	ALA B 156	32.416	-3.655	26.210	1.00 52.43
	1130	СВ	ALA B 156	31.051	-4.259	25.941	1.00 53.56
20	1131	С	ALA B 156	32.933	-2.962	24.964	1.00 52.01
	1132	0	ALA B 156	33.714	-3.527	24.203	1.00 50.83
	1133	N	LEU B 157	32.500	-1.725	24.766	1.00 53.20
,	. 1134	CA	LEU B 157	32.907	-0.945	23.606	1.00 54.15
٥.	1135	CB	LEU B 157	32.004	0.286	23.480	1.00 59.88
25	1136	CG	LEU B 157	32.116	1.171	22.238	1.00 68.36
	1137		LEU B 157	30.749	1.785	21.941	1.00 66.20
	1138		LEU B 157	33.190	2.240	22.442	1.00 73.25
	1139	С	LEU B 157	34.376	-0.535	23.711	1.00 53.24
20	1140	0	LEU B 157	35.027	-0.250	22.709	1.00 53.64
30	1141	N	LYS B 158	34.889			1.00 48.90
	1142		LYS B 158			25.196	1.00 43.03
	1143	CB	LYS B 158	36.395	0.368	26.632	1.00 51.76
	1144	CG	LYS B 158	37.738		27.006	1.00 50.73
25	1145	CD	LYS B 158	37.553		28.020	1.00 59.64
33	1146	CE	LYS B 158	36.717		29.233	1.00 62.25
	1147	NZ	LYS B 158	36.406	2.801	30.175	1.00 58.23
	1148	C	LYS B 158	37.174	-1.374	24.983	1.00 38.44
	1149	0	LYS B 158	38.192	-1.288	24.304	1.00 36.00
40	1150	N	LEU B 159	36.784		25.566	1.00 39.17
40	1151	CA	LEU B 159	37.530	-3.755	25.432	1.00 39.21
	1152	CB	LEU B 159	36.780		26.116	1.00 46.03
	1153	CG	LEU B 159	36.840		27.635	1.00 49.65
	1154	CDI	LEU B 159	35.775	-5.991	28.124	1.00 52.44

	1155	CD2	LEU	В	159	38.222	-5.492	28.034	1.00	50.53
	1156	С	LEU	В	159	37.729	-4.121	23.964	1.00	38.04
	1157	0	LEU	В	159	38.792	-4.599	23.576	1.00	32.72
	1158	N	ILE	В	160	36.692	-3.913	23.157	1.00	39.18
5	1159	CA	ILE	В	160	36.757	-4.219	21.732	1.00	39.26
	1160	СВ	ILE	В	160	35.382	-4.045	21.062	1.00	29.65
	1161	CG2	: ILE	В	160	35.493	-4.272	19.559	1.00	21.54
	1162	CG1	ILE	В	160	34.383	-5.027	21.668	1.00	33.17
	1163	CD1	ILE	В	160	32.981	-4.844	21.155	1.00	27.59
10	1164	С	ILE	В	160	37.767	-3.303	21.042	1.00	42.75
	1165	0	ILE	В	160	38.630	-3.767	20.304	1.00	41.60
	1166	N	SER	В	161	37.662	-2.001	21.283	1.00	47.98
	1167	CA	SER	В	161	38.593	-1.055	20.678	1.00	52.98
	1168	CB	SER	В	161	38.154	0.387	20.942	1.00	51.83
15	1169	OG	SER	В	161	36.966	0.699	20.235	1.00	47.45
	1170	С	SER	В	161	39.987	-1.270	21.244	1.00	54.93
	1171	0	SER	В	161	40.862	-0.420	21.103	1.00	59.36
	1172	N	GLN	В	162	40.183	-2.407	21.902	1.00	54.75
	1173	CA	GLN	В	162	41.471	-2.748	22.480	1.00	57.55
20	1174	CB	GLN	В	162	41.327	-3.031	23.971	1.00	57.42
	1175	CG	GLN	В	162	42.644	-3.337	24.667	1.00	59.30
	1176	CD			162	43.554	-2.129	24.738	1.00	61.11
	1177		GLN				-1.555	23.716		65.88
	1178	NE2	GLN	B	162	.43.923	-1.738	25.951	1.00	72.94
25	1179	С	GLN			41.989	-3.987	21.764	1.00	60.23
	1180	0	GLN	В	162	43.147	-4.047	21.358	1.00	61.01
	1181	N	ASP	В	163	41.120	-4.980	21.616	1.00	61.53
	1182	CA	ASP			41.482	-6.208	20.925	1.00	59.20
20	1183	СВ	ASP			40.345	-7.229	21.037	1.00	59.79
30	1184		ASP			40.090	-7.668	22.465	1.00	63.02
	1185		ASP			40.045	-6.796	23.354	1.00	72.81
	1186		ASP			39.924	-8.883	22.701	1.00	61.86
	1187	С	ASP			41.730	-5.850	19.459	1.00	57.70
0.5	1188	0	ASP			42.537	-6.482	18.782	1.00	55.82
35	1189	N	VAL			41.025	-4.828	18.981	1.00	57.73
	1190	CA	VAL			41.160	-4.365	17.606	1.00	59.37
	1191	СВ	VAL			40.087	-3.332	17.249	1.00	55.59
	1192		VAL			40.362	-2.753	15.865		47.40
40	1193		VAL			38.724		17.285	1.00	51.18
40	1194	C	VAL			42.504	-3.694	17.443	1.00	62.08
	1195	0	VAL			43.213	-3.914	16.461		65.19
	1196	N	LEU				-2.853	18.411		63.92
	1197	CA	LEU	В	165	44.104	-2.142	18.394	1.00	62.86

	1198	CE	LEU B 165	44.14	3 -1.140	19.547	1.00 45.47
	1199	CG	LEU B 165	45.282	2 -0.128	19.554	1.00 40.70
	1200	CD	1 LEU B 165	44.79	1.202	20.101	1.00 39.99
	1201	. CD	2 LEU B 165	46.42	4 -0.682	20.377	1.00 39.90
5	1202	С	LEU B 165	45.218	3 -3.174	18.526	1.00 63.35
	1203	0	LEU B 165	46.195	5 -3.143	17.778	1.00 63.16
	1204	N	ASP B 166	45.053	3 -4.099	19.466	1.00 64.85
	1205	CA	ASP B 166	46.029	-5.161	19.678	1.00 65.80
	1206	СВ	ASP B 166	45.736	5 -5.902	20.983	1.00 71.82
10	1207	CG	ASP B 166	46.139	-5.108	22.204	1.00 70.86
	1208	OD	1 ASP B 166	45.691	-3.950	22.338	1.00 65.25
	1209	OD	2 ASP B 166	46.904	-5,642	-23.035	1.00 80.37
	1210	С	ASP B 166	45.977	-6.145	18.514	1.00 66.21
	1211	0	ASP B 166	46.435	-7.282	18.625	1.00 ,65.89
15	1212	N	ALA B 167	45.408	-5.691	17.400	1.00 66.17
	1213	CA	ALA B 167	45.280	-6.503	16.194	1.00 66.51
	1214	CB	ALA B 167	46.612	-6.539	15.449	1.00 63.12
	1215	С	ALA B 167	44.800	-7.923	16.485	1.00 67.20
	1216	. 0	ALA B 167	45.594	-8.860	16.545	1.00 64.87
20	1217	N	LYS B 168	43.493	-8.068	16.675	1.00 69.56
•	1218	CA	LYS B 168	42.891	-9.369	16.935	1.00 70.73
	1219	CB	LYS B 168	42.391	-9.467	18.371	1.00 55.74
	1220	CG	LYS B 168	43.483	-9.612	19.384	1.00 43.98
0.5	1221	CD	LYS B 168		-10.035	20.709	1.00 50.77
25	1222	CE	LYS B 168 .,	43.995	-10.341	21.712	1.00.54.71
	1223	NZ	LYS B 168	44.917		21.875	1.00 56.54
	1224	С	LYS B 168	41.723		15.993	1.00 74.61
	1225	0	LYS B 168		-10.448	15.137	1.00 79.29
20	1226	N	ILE B 169	40.709		16.160	1.00 75.01
30	1227	CA	ILE B 169	39.541	-8.796	15.307	1.00 77.20
	1228	CB	ILE B 169		-8.822	16.137	1.00 70.32
	1229		ILE B 169		-10.003	17.095	1.00 64.44
	1230		ILE B 169	38.051		16.922	1.00 67.21
25	1231		ILE B 169	39.064	-7.306	18.014	1.00 62.39
35	1232	C	ILE B 169	39.571	-7.577	14.400	1.00 81.65
	1233	0	ILE B 169	39.866	-6.470	14.851	1.00 82.71
	1234	N	ASN B 170	39.298	-7.792	13.116	1.00 84.48
	1235	CA	ASN B 170	39.299	-6.699	12.153	1.00 86.01
40	1236	СВ	ASN B 170	38.780	-7.160	10.781	1.00 99.20
40	1237	CG	ASN B 170	39.291	-8.540	10.382	1.00105.24
	1238		ASN B 170	40.415	-8.921	10.713	1.00109.37
	1239		ASN B 170	38.466		9.651	1.00104.96
	1240	С	ASN B 170	38.361	-5.641	12.695	1.00 84.21

	1241	0	ASN B	170	37.397	-5.960	13.385	1.00 83.04
	1242	N	PRO B	171	38.630	-4.364	12.407	1.00 84.49
	1243	CD	PRO B	171	39.617	-3.766	11.493	1.00 86.08
	1244	CA	PRO B	171	37.708	-3.355	12.931	1.00 84.63
5	1245	CB	PRO B	171	38.340	-2.045	12.469	1.00 86.37
	1246	CG	PRO B	171	38.976	-2.436	11.164	1.00 86.68
	1247	C	PRO B	171	36.336	-3.610	12.306	1.00 82.79
	1248	0	PRO B	171	35.323	-3.051	12.726	1.00 82.76
	1249	N	GLY B	172	36.328	-4.480	11.299	1.00 80.64
10	1250	CA	GLY B	172	35.100	-4.828	10.613	1.00 81.32
	1251	С	GLY B	172	34.411	-6.036	11.219	1.00 81.29
	1252	0	GLY B	172	33.278	-6.351	10.859	1.00 83.71
	1253	N	ASP B	173	35.094	-6.722	12.130	1.00 79.07
٠	1254	CA	ASP B	173	34.527	-7.890	12.795	1.00 75.74
15	1255	CB	ASP B	173	35.627	-8.696	13.487	1.00 85.90
	1256	CG	ASP B	173	36.308	-9.665	12.553	1.00 90.56
	1257	OD1	ASP B	173	36.641	-9.260	11.421	1.00 93.25
•	1258	OD2	ASP B	173	36.514	-10.830	12.952	1.00 92.57
	1259	С	ASP B	173	33.481	-7.464	13.822	1.00 70.25
20	1260	0	ASP B	173	32.727	-8.288	14.343	1.00 68.50
	1261	N	ILE B	174	33.444	-6.169	14.114	1.00 65.51
	1262	CA	ILE B	174	32.486	-5.628	15.064	1.00 60.45
	1263	СВ	ILE B	174	32.687	-4.119	15.234	1.00 48.40
	1264	. CG2	ILE B	174	31.684	-3.562	16.226	1.00 46.12
25	1265	CG1	ILE B	174	34.115	-3.851	15.702	1.00 44.86
•	1266	CD1	ILE B	174	34.461	-2.387	15.797	1.00 31.07
	1267	С	ILE B		31.077	-5.886	14.549	1.00 58.37
	1268	0	ILE B	174	30.679	-5.344	13.524	1.00 58.27
	1269	N	THR B	175	30.327	-6.719	15.261	1.00 55.65
30	1270	CA	THR B				14.869	1.00 53.67
	1271		THR B		28.897	-8.435	14.236	1.00 57.15
	1272		THR B		29.168	-9.429	15.230	1.00 55.78
	1273	•	THR B		29.932			1.00 49.80
a =	1274	С	THR B 1		28.084			1.00 52.38
35	1275	0	THR B 1	L75	28.577	-6.835	17.217	1.00 52.43
	1276	N	GLU B 1		26.784	-7.232	15.938	1.00 51.31
	1277	CA	GLU B 1		25.895	-7.261	17.089	1.00 48.46
	1278	СВ	GLU B 1	176	24.434	-7.240	16.643	1.00 37.51
	1279	CG	GLU B 1		23.950		16.281	1.00 45.01
40	1280	CD	GLU B 1		22.474	-5.813	15.956	1.00 45.89
	1281				21.690		16.615	1.00 42.92
	1282		GLU B 1		•		15.051	1.00 34.90
	1283	С	GLU B 1	.76	26.187	-8.519	17.893	1.00 49.50
						*		

	1284	0	GLU	B 176	26.038	8 -8.544	19.113	1.00	49.76
	1285	N	GLU	в 177	26.613	-9.563	17.192	1.00	48.42
	1286	CA	GLU	в 177	26.950	-10.820	17.836	1.00	48.94
	1287	СВ	GLU	В 177	27.318	3 -11.868	16.779	1.00	63.07
5	1288	CG	GLU	в 177	27.685	-13.239	17.350	1.00	72.68
	1289	CD	GLU	В 177	28.766	-13.953	16.545	1.00	76.09
•	1290	OE	1 GLU	B 177	29.081	-15.121	16.869	1.00	77.97
	1291	OE	2 GLU	В 177	29.309	-13.346	15.595	1.00	76.21
	1292	С	GLU	в 177	28.149	-10.576	18.754	1.00	47.13
. 10	1293	0	GLU	В 177	28.129	-10.926	19.934	1.00	43.82
	1294	N	LEU	В 178	29.189	-9.960	18.199	1.00	46.13
	1295	CA	LEU	В 178	30.416	-9.678	18.938	1.00	41.18
	1296	CB	LEU	в 178	31.444	-9.015	18.011	1.00	31.24
	1297			В 178	32.881	-8.843	18.521	1.00	29.48
15	1298		l LEU		33.762	-8.385	17.378	1.00	32.21
	1299	CD2	2 LEU	B 178	32.940	-7.834	19.650	1.00	38.13
	1300	С		В 178	30.176	-8.805	20.166	1.00	41.26
	1301	0		B 178			21.286	1.00	44.23
20	1302	N		B 179	29.669	-7.591	19.954	1.00	37.47
20	1303	CA		В 179	29.395		21.053	1.00	33.95
	1304	СВ		B 179	28.502		20.592	1.00	25.86
	1305		? ILE 1		28.071		21.783		27.50
	. 1306		. ILE I		29.267		19.617		24.58
25	1307		ILE I		28.434		19.007		16.92
25	1308	С		3 179	28.687				36.09
	1309	0	ILE E		28.901		23.367		36.52
	1310	N	GLY E		27.849		21.821		37.19
	1311	CA	GLY E		27.108	-9.120		•	34.45
30	1312	C	GLY F			-10.057			33.00
50	1313	0	GLY E			-10.390	24.766		32.59
	1314 1315	N	ASN E			-10.491			35.65
	1316	CA CB	ASN E			-11.388			34.95
	1317	CG	ASN E			-12.153	22.784		30.99
35	1318		ASN E			-13.010	21.838		27.11
35	1319		ASN B			-13.735	22.251		30.62
	1320	C	ASN B			-12.943	20.557		34.99
	1321	0	ASN B			-10.617	24.724	1.00	
	1322	N				-11.224	25.486	1.00	
40	1323	CA	TYR B			-9.288 -9.456	24.684	1.00	
	1324	CB	TYR B			-8.456	25.552	1.00	
	1325	CG	TYR B		32.323		24.742	1.00	
	1326		TYR B			-7.857 -8.829	23.974		30.62
	1020	001	TIV D	102	33.411	-8.828	22.976	1.00	JI.56

	1327	CE1	TYR	. В	182	34.533	-9.256	22.247	1.00	31.15
	1328	CD2	· TYR	В	182	34.796	-7.325	24.229	1.00	32.17
	1329	CE2	TYR	В	182	35.921	-7.740	23.507	1.00	29.49
	1330	CZ	TYŖ	В	182	35.783	-8.705	22.520	1.00	30.88
5	1331	ОН	TYR	В	182	36.898	-9.105	21,814	1.00	38.87
	1332	С	TYR	В	182.	30.871	-7.814	26.689	1.00	30.63
	1333	0	TYR	В	182	31.455	-7.108	27.507	1.00	27.81
	1334	N	LEU	В	183	29.565	-8.055	26.736	1.00	33.68
	1335	CA	LEU	· в	183 .	28.722	-7.510	27.795	1.00	39.37
10	1336	СВ	LEU	В	183	27.281	-7.389	27.298	1.00	39.69
	1337	CG	LEU	· B	183	27.086	-6.546	26.040	1.00	35.29
	1338	CD1	LEU	В	183	25.629	-6.594	25.618	1.00	30.83
	1339	CD2	LEU	В	183	27.525	-5.121	26.308	1.00	36.26
	1340	С	LEU	В	183	28.780	-8.422	29.030	1.00	40.34
15	1341	0	LEU	В	183	29.084	-9.610	28.915	1.00	39.87
	1342	N	PHE	В	184	28.490	- 7.873	30.206	1.00	38.84
	1343	CA	PHE	В	184	28.532	-8.659	31.437	1.00	37.83
•	1344	СВ	PHE	В	184	28.026	-7.843	32.633	1.00	31.19
	1345	CG	PHE	В	184	28.751	-6.538	32.843	1.00	28.22
20	1346	CD1	PHE	В	184	30.068	-6.377	32.436	1.00	30.85
	1347	CD2	PHE	В	184	28.115	-5.474	33.481	1.00	33.99
	1348	CE1	PHE	В	184	30.736	-5.175	32.663	1.00	24.17
	1349	CE2	PHE	В	184	28.778	-4.268	33.713	1.00	21.76
	1350	CZ	PHE	В	184	30.087	-4.120	33.305	1.00	18.36
25	1351	С	PHE	В	184	27.697	-9.929	31.319	1.00	36.97
	1352	0	PHE	В	184	27.947	-10.914	32.014	1.00	32.04
	1353	N	THR	В	185	26.704	-9.903	30.441	1.00	38.47
	1354	CA	THR	В	185	25.841	-11.059	30.243	1.00	42.41
	1355	СВ	THR	В	185	24.478	-10.625	29.741	1.00	34.61
30	1356	OG1	THR	В	185	24.651	-9.691	28.671	1.00	41.28
	1357	CG2	THR	В	185	23.696	-9.975	30.853	1.00	34.33
	1358	С	THR	В	185	26.423	-12.052	29.248	1.00	44.70
	1359	0	THR	В	185	25.700	-12.896	28.720	1.00	41.53
	1360	N	GLN	В	186	27.728	-11.951	29.008	1.00	48.74
35	1361	CA	GLN	В	186	28.438	-12.826	28.074	1.00	49.59
	1362	CB	GLN	В	186	29.790	-12.227	27.736	1.00	45.10
	1363	CG	GLN	В	186	30.776	-12.389	28.875	1.00	43.93
	1364	CD	GLN	В	186	32.116	-11.753	28.593	1.00	47.95
	1365	OE1	GLN	В	186	32.249	-10.530	28.593	1.00	50.02
40	1366	NE2	GLN	В	186	33.119	-12.583	28.342	1.00	38.99
	1367	C	GLN				-14.203		1.00	51.53
	1368	0	GLN	В	186	29.115	-15.130	27.996	1.00	55.42
	1369	N	HIS	В	187	28.409	-14.320	29.977	1.00	50.40

	1370	CA	HIS	в 187	,	28.598	3 -15.565	30.708	1.00	49.57
	1371	СВ	HIS	B 187	,	28.77	3 -15.243	32.190	1.00	42.89
	1372	CG	HIS	в 187	,	29.843	l -14.223	32.442	1.00	49.91
	1373	CD2	2 HIS	В 187	,	29.80	L -13.022	33.068	1.00	49.67
5	1374	ND:	l HIS	B 187	,	31.127	7 -14.361	31.962	1.00	43.80
	1375	CE	l HIS	в 187	·	31.833	3 -13.289	32.278	1.00	48.87
	1376	NE	2 HIS	B 187	,	31.053	3 -12.460	32.949	1.00	46.70
	1377	С	HIS.	B 187	,	27.439	9 -16.521	30.487	1.00	52.33
	1378	0	HIS	B 187	'	27.636	5 -17.718	30.286	1.00	53.97
10	1379	N	LEU	в 188	1	26.226	5 -15.992	30.514	1.00	54.52
	1380	CA	LEU	в 188		25.051	-16.813	30.289	1.00	51.83
	1381	СВ	LEU	в 188		23.789	-15.984	30.549	1.00	44.55
	1382	CG	LEU	в 188		23.659	-15.395	31.962	1.00	47.65
	1383	CD1	LEU	в 188		22.452	2 -14.467	32.039	1.00	49.93
15	1384	CD2	LEU	в 188	•	23.537	-16.520	32.980	1.00	56.89
	1385	С	LEU	в 188		25.085	-17.310	28.838	1.00	52.44
	1386	.0	LEU	B 188		25.560	-16.611	27.946	1.00	53.35
	1387	N	PRO	B 189		24.594	-18.532	28.590	100	51.33
	1388	CD	PRO	B 189		23.882	-19.388	29.549	1.00	51.94
20	1389	CA	PRO	B 189		24.565	-19.127	27.244	1.00	49.93
	1390	CB	PRO	B 189	,	23.822	-20.442	27.463	1.00	51.02
	1391	CG	PRO	B 189		22.944	-20.139	28.642	1.00	52.36
	1392	С	PRO	В 189	<i>:.</i> .	23.878	-18.244	26.210	1.00	46.59
	1393	0	PRO	в 189	•	22.834	-17.661	26.482	1.00	45.97
25	1394	N	LYS	В 190		24.451	-18.166	25.016	1.00	42.50
	1395	CA	LYS	B 190		23.889	-17.315	23.977	1.00	39.80
	1396	CB	LYS	B 190		. 24.439	-17.688	22.596	1.00	36.33
	1397	CG		В 190			-17.235	22.345	1.00	38.65
20	1398	CD		В 190		26.252	-17.384	20.871	1.00	42.37
30	1399	CE		В 190			-17.183	20.632	1.00	50.39
	1400	NZ		В 190			-15.806	20.958	1.00	58.82
	1401	С		В 190			-17.219			39.26
	1402	0 -		B 190			-16.115	23.940		39.95
25	1403	N		3 191			-18.337	23.777	1.00	40.10
35	1404	CA	ASP I				-18.235	23.658		39.42
	1405	CB	ASP I				-19.543	23.098		39.52
	1406	CG	ASP I				-20.721	24.060		44.32
	1407		ASP I				-21.170	24.306	1.00	39.96
40	1408		ASP F				-21.200		1.00	
40	1409	C	ASP E				-17.804	24.936		39.16
•	1410	0	ASP E				-17.604	24.922		41.35
	1411	N	LEU E				-17.632			37.21
	1412	CA	LEU E	3 192		19.589	-17.218	27.294	1.00	34.43

	1413	СВ	LEU	в 192	19.877	-18.258	28.397	1.00 26.76
	1414	CG	LEU	В 192	19.100	-19.585	28.315	1.00 23.82
	1415	CD1	LEU	В 192	19.659	-20.569	29.310	1.00 16.92
	1416	CD2	LEU	в 192	17.607	-19.345	28.582	1.00 16.92
5	1417	С	LEU	в 192	20.024	-15.826	27.761	1.00 34.24
	1418	0	LEU	в 192	19.508	-15.310	28.748	1.00 38.50
	1419	N	ARG	в 193	20.957	-15.221	27.029	1.00 30.50
	1420	CA	ARG	в 193	21.484	-13.900	27.358	1.00 29.14
	1421	СВ	ARG	в 193	22.587	-13.507	26.377	1.00 23.71
10	1422	ÇG	ARG	в 193	23.838	-14.307	26.522	1.00 24.21
	1423	CD	ARG	в 193	24.862	-13.896	25.494	1.00 20.84
	1424	NE	ARG	в 193	26.131	-14.599	25.681	1.00 31.16
	1425	CZ	ARG	в 193	27.191	-14.455	24.890	1.00 37.18
	1426	NH1	ARG	в 193	27.141	-13.630	23.846	1.00 39.87
15	1427	NH2	ARG	в 193	28.303	-15.131	25.147	1.00 37.17
	1428	С	ARG	в 193	20.483	-12.756	27.415	1.00 28.97
	1429	0	ARG :	В 193	20.638	-11.853	28.225	1.00 29.31
•	1430	N	ASP :	В 194	19.465	-12.764	26.566	1.00 24.43
	1431	CA	ASP	В 194	18.520	-11.660	26.588	1.00 26.20
20	1432	СВ	ASP :	В 194	18.180	-11.217	25.157	1.00 21.25
	1433	CG	ASP 1	В 194	19.413	-10.763	24.361	1.00 25.14
	1434	OD1	ASP I	3 194	20.357	-10.207	24.973	1.00 16.92
	1435	OD2	ASP 1	3 194	19.427	-10.948	23.119	1.00 30.59
•	1436	C	ASP I	3 194	17.241	-11.990	27.344	1.00 24.70
25	1437	0	ASP I	3 194	16.638	-13.043	27.133	1.00 31.23
٠.	1438	N	PRO I	3 195	16.811	-11.088	28.242	1.00 19.04
	1439	CD	PRO I	3 195	17.403	-9.779	28.558	1.00 16.92
	1440	CA	PRO E	3 195	15.593	-11.299	29.024	1.00 22.28
	1441	СВ	PRO I	3 195	15.552	-10.077	29.935	1.00 21.56
30	1442	CG	PRO I	3 195	16.229	-9.044	29.139	1.00 18.86
	1443	С	PRO E	3 195	14.392	-11.371	28.110	1.00 24.96
	1444	0	PRO E	3 195	14.345	-10.680	27.101	1.00 30.51
	1445	N	ASP E	3 196	13.431	-12.217	28.450	1.00 22.33
	1446	CA	ASP E	196	12.237	-12.347	27.631	1.00 21.67
35	1447	CB	ASP E	196	11.826	-13.808	27.522	1.00 21.17
	1448	CG	ASP E		12.875	-14.636	26.849	1.00 35.32
	1449		ASP E			-15.133	27.550	1.00 31.80
				196	12.808	-14.767	25.609	1.00 44.56
	1451		ASP E		11.116	-11.525	28.225	1.00 22.00
40	1452		ASP E			-11.363	27.633	1.00 22.34
	1453				11.381	-10.999	29.409	1.00 24.46
	1454			197		-10.174	30.104	1.00 22.14
	1455	CB	LEU B	197	9.336	-11.036	30.748	1.00 16.92

	1456	CG	LEU	В	197	8.462	-10.340	31.797	1.00	16.92
	1457	CDI	LEU	В	197	7.828	-9.10	31.228	1.00	18.26
	1458	CD2	LEU	В	197	7.396	-11.27	32.273	1.00	23.97
	1459	С	LEU	JВ	197	11.163	-9.394	31.163	1.00	24.32
5	1460	0	LEU	В	197	12.064	-9.913	31.809	1.00	31.10
	1461	N	ILE	В	198	10.806	-8.128	31.312	1.00	25.23
	1462	CA	ILE	В	198	11.419	-7.301	32.327	1.00	23.49
	1463	СВ	ILE	В	198	12.252	-6.163	31.728	1.00	16.92
	1464	CG2	LLE	В	198	12.760	-5.255	32.837	1.00	16.92
10	1465	CG1	. ILE	В	198	13.434	-6.755	30.956	1.00	19.52
	1466	CD1	ILE	В	198	14.494	-5.751	30.554	1.00	16.92
	1467	С	ILE	В	198	10.312	-6.750	33.205	1.00	26.00
	1468	0	ILE	В	198	9.458	-5.983	32.760	1.00	23.12
	1469	N	ILE	В	199	10.336	-7.191	34.457	1.00	30.16
15	1470	CA	ILE	В	199	9.361	-6.808	35.457	1.00	31.89
	1471	СВ	ILE	В	199	9.169	-7.966	36.461	1.00	31.40
	1472	CG2	ILE	В	199	8.241	-7.539	37.597	1.00	35.99
	1473	CG1	ILE	В	199	8.635	-9.194	35.709	1.00	30.96
	1474	CD1	ILE	В	199	8.432	-10.422	36.562	1.00	25.50
20	1475	С	ILE	В	199	9.797	-5.547	36.196	1.00	30.27
	1476	0	ILE	В	199	10.973	-5.382	36.511	1.00	30.43
	1477	N	ARG	В	200	8.843	-4.657	36.450	1.00	29.84
	1478	CA	ARG	В	200	9.102	-3.413	37.167	1.00	34.70
	1479	CB	ARG	В	200	9.192	-2.235	36.190	1.00	38.24
25	1480	CG	ARG	В	200	9.649	-0.923	36.828	1.00	38.39
	1481	CD	ARG	В	200	11.047	-1.036	37.439	1.00	41.65
	1482	NE	ARG	В	200	11.489	0.171	38.148	1.00	34.53
	1483	CZ	ARG	В	200	11.935	1.290	37.572	1.00	18.77
	1484	NH1	ARG	В	200	12.014	1.399	36.252	1.00	16.92
30	1485	NH2	ARG	В	200	12.314	2.307	38.326	1.00	18.24
		С	ARG	В	200		-3.211	38.145	1.00	35.76
	1487	0	ARG			6.783	-3.252	37.756	1.00	33.19
	1488	N	THR			8.277	-3.001	39.414	1.00	38.28
~~	1489	CA	THR			7.262	-2.835	40.449	1.00	37.05
35	1490	CB	THR			7.586			1.00	16.92
	1491		THR			8.943	-3.503	42.070	1.00	29.17
	1492		THR	В	201	7.417	-5.174	41.315	1.00	19.67
	1493	С	THR	В	201	7.102		40.940	1.00	39.68
4.0	1494	0	THR			7.833	-0.509	40.522	1.00	41.56
40	1495	N	SER			6.129		41.826	1.00	41.87
	1496	CA	SER				0.101			39.34
	1497	CB	SER					42.992	1.00	19.15
	1498	OG	SER	В	202	6.945	1.980	43.512	1.00	39.12

	1499	С	SER	B 202	5.190	1.151	41.538	1.00	40.05
	1500	0	SER	B 202	4.920	2.262	41.995	1.00	47.17
	1501	N	GLY	B 203	4.922	0.811	40.281	1.00	38.45
	1502	CA	GLY	B 203	4.287	1.762	39.377	1.00	37.08
5	1503	С	GLY	B 203	5.271	2.563	38.534	1.00	35.70
	1504	0	GLY	B 203	4.886	3.461	37.787	1.00	37.31
	1505	N	GLU	B 204	6.550	2.231	38.654	1.00	29.52
	1506	CA	GLU	B 204	7.586	2.917	37.908	1.00	28.07
	1507	СВ	GLU.	B 204	8.952	2.653	38.538	1.00	26.30
10	1508	CG	GLU	B 204	9.236	3.482	39.779	1.00	48.79
	1509	CD	GLU,	B 204	8.973	4.961	39.556	1.00	50.97
	1510	OE1	GLU	B 204	7.849	5.419	39.869	1.00	42.50
	1511	OE2	GLU	B 204	9.877	5.663	39.055	1.00	50.61
	1512	С	GLU	B 204	7.616	2.477	36.462	1.00	29.34
15	1513	0	GLU	B 204	7.878	1.317	36.175	1.00	34.97
	1514	N	LEU.	B 205	7.354	3.408	35.552	1.00	24.91
	1515	CA	LĘU	B 205	7.371	3.119	34.120	1.00	25.98
	1516	CB	LEU	В 205	6.104	3.666	33.470	1.00	25.92
	1517	CG	LEU	В 205	4.825	3.056	34.050	1.00	23.50
20	1518	CD1	LEU	B 205	3.610	3.785	33.547	1.00	16.92
	1519	CD2	LEU	B 205	4.753	1.600	33.668	1.00	30.67
	1520	С	LEU	B 205	8.607	3.733	33.472	1.00	28.56
	1521	0	LEU	В 205	8.526	4.382	32.441	1.00	29.61
	1522	N	AŖG	B 206	9.758	3.,533	34.093	1.00	33.33
25	1523	CA	ARG	B 206	10.992	4.075	33.561	1.00	37.25
	1524	СВ	ARG	B 206	11.776	4.826	34.645	1.00	42.74
	1525	CG	ARG	B 206	10.936	5.391	35.782	1.00	40.30
	1526	CD		B 206	11.792	6.156	36.799	1.00	44.32
	1527	NE		В 206	12.921				65.13
30	1528			B 206	13.705	5.748	38.324	1.00	69.76
	1529			B 206	13.483	6.904	38.937	1.00	76.09
	1530			В 206	14.714	4.974	38.727	1.00	74.71
	1531	С		В 206	11.815			1.00	42.39
25	1532	0		B 206	11.384		33.228	1.00	42.90
35	1533	N		B 207	13.005		32.592	1.00	44.87
	1534	CA		B 207	13.887	2.114	32.150	1.00	48.66
	1535	CB		B 207	14.442	2.437		1.00	63.61
	1536	CG		B 207	13.391	2.281	29.657	1.00	70.49
40	1537		LEU 1		13.973	2.698	28.321	1.00	76.92
40	1538		LEU 1		12.916	0.827	29.600		75.21
	1539	C		3 207	15.001	1.932	33.175	1.00	47.29
	1540	0	LEU I		15.499	0.821	33.372		47.01
	1541	N	SER I	3 208	15.373	3.027	33.833	1.00	42.15

	1542	CA	SER E	3 208	16.407	3.001	34.866	1.00 32.73
	1543	СВ	SER E	208	15.926	2.180	36.062	1.00 33.90
	1544	OG	SER E	208	14.588	2.494	36.396	1.00 24.12
	1545	С	SER E	208	17.752	2.451	34.404	1.00 28.39
5	1546	0	SER B	208	18.480	1.841	35.193	1.00 29.45
	1547	N	ASN B	209	18.071	2.652	33.128	1.00 26.85
	1548	CA	ASN B	209	19.348	2.212	32.561	1.00 27.50
	1549	СВ	ASN B	209	20.468	3.114	33.127	1.00 16.92
	1550	CG	ASN B	209	21.836	2.862	32.494	1.00 22.61
10	1551	OD:	L ASN B	20,9	21.954	2.602	31.300	1.00 26.46
	1552	ND	2 ASN B	209	22.880	2.972	33.303	1.00 20.95
	1553	С	ASN B	209	19.645	0.730	32.814	1.00 32.21
	1554	0	ASN B	209	20.801	0.317	32.892	1.00 34.11
	1555	N	PHE B	210	18.592	-0.074	32.915	1.00,34.72
15	1556	CA	PHE B	210	18.754	-1.504	33.172	1.00 30.65
	1557	CB	PHE B	210	17.651	-1.991	34.122	1.00 21.62
	1558	CG	PHE B	210	17.790	-3.433	34.537	1.00 28.42
	1559	CD1	PHE B	210	18.932	-3.875	35.195	1.00 32.07
	1560	CD2	PHE B	210	16.769	-4.344	34.283	1.00 24.66
20	1561	CE1	PHE B	210	19.057	-5.194	35.594	1.00 22.48
	1562	CE2	PHE B	210	16.884	-5.663	34.677	1.00 24.33
	1563	CZ	PHE B	210	18.032	-6.090	35.334	1.00 18.91
	1564	С	PHE B	210	18.721	-2.309	31.881	1.00 30.28
	1565	O	PHE B	210	17.778	-2.197	31.101	1.00 26.90
25	1566	N	LEU B	211	19.759	-3.117	31.673	1.00 31.38
	1567	CA	LEU B		19.888	-3.959	30.484	1.00 30.02
	1568	СВ	LEU B		19.093	-5.253	30.661	1.00 19.94
	1569	CG	LEU B		19.715	-6.354	31.512	1.00 17.90
20	1570		LEU B		18.863	-7.623	31.409	1.00 17.79
30	1571		LEU B		21.132	-6.619	31.024	1.00 28.12
	1572	С	LEU B		19.454	-3.287	29.183	1.00 33.52
	1573	0	LEU B		18.659	-3.841	28.414	1.00 35.70
	1574	N	PRO B		19.994	-2.094	28.902	1.00 34.82
25	1575	CD	PRO B		21.175	-1.502	29.547	1.00 34.05
35	1576	CA	PRO B		19.648	-1.359	27.684	1.00 31.21
	1577	CB	PRO B		20.608	-0.183	27.724	1.00 30.61
	1578		-PRO B		21.801	-0.762	28.411	1.00 33.84
	1579	С	PRO B		19.777	-2.188	26.400	1.00 28.88
40	1580	0	PRO B		18.862	-2.209	25.578	1.00 28.95
40	1581	N	TRP B		20.905	-2.878	26.241	1.00 32.89
	1582	CA	TRP B		21.151	-3.705	25.062	1.00 34.16
	1583	СВ	TRP B		22.653	-3.980	24.928	1.00 36.50
	1584	CG	TRP B	213	23.024	-4.885	23.779	1.00 40.25

	11 0 0010										
	1585	CD	2 TRE	E	213		23.654	-4.494	22.559	1.00	41.82
	1586	CE	2 TRE	, E	213		23.825	-5.664	21.782	1.00	42.56
	1587	CE	3 TRE	E	213		24.096	-3.266	22.043	1.00	36.15
	1588	CD	1 TRE	E	213		22.837	-6.241	23.695	1.00	34.48
5	1589	NE.	1 TRE	B	213		23.317	-6.713	22.500	1.00	35.36
	1590	CZ	2 TRE	B	213		24.421	-5.640	20.516	1.00	41.79
	1591	CZ	3 TRE	В	213		24.687	-3.244	20.783	1.00	44.66
	1592	CH	2 TRF	В	213		24.845	-4.426	20.035	1.00	41.35
	1593	С	TRE	В	213		20.375	-5.034	25.026	1.00	31.31
10	1594	0	TRP	В	213		19.551	-5.252	24.140	1.00	28.47
	1595	N	GLN	В	214		20.644	-5.922	25.978	1.00	29.42
	1596	CA	GLN	В	214		19.975	-7.220	26.027	1.00	27.98
	1597	СВ	GLN	В	214		20.420	-7.989	27.277	1.00	29.16
	1598	CG	GLN	В	214		21.926	-8.184	27.438	1.00	30.26
15	1599	CD	GLN	В	214		22.631	-7.032	28.150	1.00	35.27
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	1601	NE2	GLN	В	214		22.021	-5.852	28.137	1.00	36.97
•	1602	С	GLN	В	214		18.442	-7.114	26.018	1.00	26.22
	1603	0	GLN	В	214		17.747	-7.935	25.414	1.00	26.19
20	1604	N	GLY	В	215		17.918	-6.101	26.695	1.00	24.50
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	1606	С	GLY	В	215		15.870	-5.269	25.536	1.00	20.33
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4	1608	N	ALA	В	216	,	16.671	-5.045	24.495	1.00	16.97
25	1609	CA	ALA	В	216		16.207	-4.397	23.265	1.00	17.93
	1610	CB	ALA	В	216		17.162	-4.710	22.109	1.00	17.20
	1611	С	ALA	В	216		. 14.773	-4.758	22.875	1.00	20.59
	1612	0	ALA				13.970	-3.865	22.602	1.00	23.60
20	1613	N	TYR	В	217		14.437	-6.049	22.854	1.00	24.42
30	1614	CA	TYR	В	217		13.073	-6.462	22.494	1.00	18.63
	1615	CB	TYR	В	217		13.070	-7.402	21.282	1.00	16.92
	1616	CG			217	*	13.921	-6.990	20.092	1.00	16.92
	1617		TYR				15.315		20.127	1.00	16.92
25	1618		TYR				16.092	-6.810	19.007	1.00	16.92
35	1619		TYR				13.328	-6.538	18.901	1.00	16.92
	1620		TYR				14.098	-6.230	17.779	1.00	16.92
,	1621	CZ	TYR				15.476		17.840	1.00	16.92
	1622	ОН	TYR				16.247		16.735	1.00	16.92
40	1623	С	TYR				12.326	-7.173	23.629	1.00	16.92
40	1624	0	TYR				11.433		23.380	1.00	16.92
	1625	N	SER				12.673		24.873	1.00	16.92
	1626	CA	SER						25.989	1.00	16.92
	1627	CB	SER	В	218		12.814	-7.308	27.268	1.00	23.90

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	1671	. N	THR E	3 223	3	3.729	-3.485	37.486	1.00	27.43
	1672	CA	THR E	223	3	2.747	-3.695	38.529	1.00	29.24
	1673	СВ	THR E	223	}·	, 2.922	-5.072	39.179	1.00	30.96
	1674	OG:	1 THR E	223	;	1.913	-5.255	40.173	1.00	38.54
5	1675	CG2	2 THR E	, 223		4.290	-5.188	39.834	1.00	18.62
	1676	· c	THR E	223		2.913	-2.643	39.591	1.00	31.84
	1677	0	THR E	223		3.992	-2.094	39.757	1.00	30.89
	1678	N	ASP B	224		1.842	-2.359	40.315	1.00	36.42
	1679	CA	ASP B	224	,	1.895	-1.365	41.377	1.00	40.14
10	1680	СВ	ASP B	224		0.494	-0.818	41.648	1.00	41.56
	1681	CG	ASP B	224		0.062	0.206	40.624	1.00	46.72
	1682	OD1	ASP B	224		-1.144	0.529	40.590	1.00	43.47
	1683	OD2	ASP B	224	٠.	, 0.928	0.693	39.864	1.00	54.57
	1684	С	ASP B	224		2.480	-1.939	42.667	1.00	40.48
15	1685	0	ASP B	224		3.280	-1.285	43.341	1.00	42.72
	1686	N	THR B	225		2.085	-3.163	43.002	1.00	37.47
	1687	. CA	THR B	225		2.566	-3.806	44.217	1.00	37.52
	1688	CB	THR B	225		2.344	-5.347	44.183	1.00	32.35
	1689	OG1	THR B	225		2.884	-5.882	42.971	1.00	45.94
20	1690	CG2	THR B	225		0.853	-5.686	44.282	1.00	27.82
	1691	С	THR B	225		4.045	-3.520	44.459	1.00	36.64
	1692	0	THR B			4.853	-3.545	43.525	1.00	32.74
	1693	N	LEU B			4.374	-3.221	45.718	1.00	40.20
٥٣	1694	CA	•				-2.934	46.126	1.00	37.95
25	1695	CB	LEU B			5.768	-2.291	47.511	1.00	27.85
	1696	CG	LEU B			5.116				16.92
	1697		LEU B				-0.129		1.00	20.23
	1698		LEU B				-1.053		1.00	16.92
20	1699	С	LEU B			6.536	-4.225			34.39
30	1700		LEU B			6.008		46.476	1.00	33.65
	1701	N	TRP B			7.815	-4.129	45.807	1.00	27.74
	1702	CA	TRP B			8.661	-5.302	45.736	1.00	26.44
	1703	CB	TRP B			10.104	-4.903	45.490	1.00	16.92
35	1704	CG	TRP B			10.987	-6.092	45.465	1.00	
33	1705 1706		TRP B			10.954	-7.160	44.513	1.00	
	1707		TRP B			11.975	-8.066	44.869	1.00	
	1708		TRP B			10.167	-7.437		1.00	
	1709		TRP B			11.990	-6.386	46.338	1.00	
40		•	TRP B				-7.570	45.989	1.00	
-10	1710 1711		TRP B			12.231	-9.229		1.00	
	1712		TRP B			10.422	-8.590		1.00 2	
	1713		TRP B						1.00	
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	1716	CD	PRO E	228	9.315	-4.485	48.571	1.00	32.12
	1717	CA	PRO E	228	8.816	-6.738	49.281	1.00	33.56
5	1718	CB	PRO E	228	9.021	-5.818	50.469	1.00	30.46
	1719	CG	PRO E	228	9.943	-4.792	49.913	1.00	31.06
	1720	С	PRO E	228	7.511	-7.501	49.359	1.00	36.50
	1721	0	PRO. B	228	7.412	-8.499	50.067	1.00	39.78
	1722	N	ASP B	229	6.513	-7.023	48.620	1.00	38.84
10	1723	CA	ASP B	229	5.195	-7.645	48.581	1.00	37.34
	1724	CB	ASP B	229	4.107	-6.564	48.528	1.00	34.82
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	1726		1 ASP B		3.018	-5.009	49.953	1.00	49.11
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15	1728	С	ASP B		5.042	-8.564	47.370	1.00	35.86
	1729		ASP B		3.979		47.164	1.00	38.47
	1730	N	PHE B		6.100		46.575		31.52
	1731	CA	PHE B		6.047	-9.533	45.371		29.58
20	1732	CB	PHE B		7.152	-9.127	44.382		30.24
20	1733	CG	PHE B		6.750		42.922		39.74
	1734		L PHE B		5.791	-8.388	42.380		35.52
•	1735		PHE B			-10.171	42.082		36.37
	1736 1737		PHE B		5.447	-8.456	41.021		28.22
25	1738	CZ	PHE B			-10.247	40.727		28.28
	1739	C	PHE B		6.066	-9.386	40.199		28.51
	1740	0	PHE B			-11.020 -11.582	45.695		31.09
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	1742	CA	ASP B			-13.056	46.265		30.72
30	1743	СВ	ASP B			-13.288	47.001		35.43
	1744	CG		231		-12.714			
	1745	OD1	ASP B			-12.730			51.61
	1746		ASP B			-12.247			31.99
	1747	С	ASP B	231		-13.930		1.00	
35	1748	0	ASP B	231		-13.432		1.00	
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	1750	CA	GLU B	232	4.825	-16.192	44.115	1.00	
	1751	СВ	GLU B	232			44.656	1.00	
	1752	CG	GLU B	232	4.652		43.577	1.00	
40	1753	CD	GLU B	232	4.506		44.129	1.00	
	1754	OE1	GLU B	232	3.511		44,825	1.00	
	1755	OE2	GLU B	232	5.385		43.863		31.43
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·	1865	C1	3 FF	PPC	2	21.55	4 -9.256	47.774	1.00 73.49
5	1866	C1	4 FF	PPC	2	22.73	1 -10.024	47.224	1.00 74.43
	1867	C1	5 FP	P C	2	20.81	6 -10.087	48.804	1.00 73.47
	1868	PA	FP	PC	2	13.81	1.633	46.280	1.00 96.03
	1869	01	A FP	P C	2	14.399	2.089	47.657	1.00 94.67
	1870	02	A FP	P C	2	13.930	2.601	45.086	1.00 95.64
10	1871	03	A FP	PC	2	12.383	3 1.423	46.754	1.00 97.67
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	1873	01	B FP	P C	2	10.986	2.923	45.165	1.00102.75
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	1875	03	B FP	P C	2	10.046	2.557	47.285	1.00101.13
15	1876	OH	2 WA	T W	1	4.773	7.298	32.511	1.00 36.80
	1877	OH	2 WA	T W	2	6.323	0.871	14.427	1.00 36.80
	1878	OH:	2 WA'	r w	3	15.515	-0.599	23.674	1.00 36.80
•	1879	OH	2 WA!	r w	4	-7.863	3.523	18.482	1.00 36.80
	1880	OH	2 WAS	r w	5	16.858	9.374	28.786	1.00 36.80
20	1881	OH2	2 WAT	r W	6	11.507	-3.595	14.868	1.00 36.80
	1882	OH2	WAT	r W	7	34.098	13.685	24.109	1.00 36.80
	1883	OH2	AW S	C M	8	-6.504	15.936	17.044	1.00 36.80
	. 1884	OH2	EAW S	' W	9	16.680	15.674	27.816	1.00 36.80
	1885	OH2	raw :	W	10	16.423	23.057	25.423	1.00 36.80
25	1886	OH2	rAW :	W	11	-0.276	12.147	0.194	1.00 36.80
	1887	OH2	WAT	W	12	41.369	13.097	17.334	1.00 36.80
	1888	OH2	TAW	W	13	22.635	10.116	22.907	1.00 36.80
	1889	OH2	TAW	W	14	15.672	1.557	26.009	1.00 36.80
	1890		WAT		15	19.186	15.106	27.885	1.00 36.80
30	1891		WAT		16	39.396	4.075	29.930	1.00 36.80
	1892	OH2	WAT	W	17	23.260	21.078	25.999	1.00 36.80
	1893	OH2	TAW	W	18	10.020	-9.291	1.405	1.00 36.80
	1894	OH2	TAW	W	19	23.088	-10.033	21.137	1.00 36.80
	1895	OH2	TAW	W	20	7.776	-6.623	10.879	1.00 36.80
35	1896	OH2	WAT	W	. 21	19.914	-3.586	15.083	1.00 36.80
	1897	OH2	TAW	W	22	-12.008	5.707	9.673	1.00 36.80
	1898	OH2	WAT	W	23	8.883	29.025	9.092	1.00 36.80
	1899		TAW		24	24.894	18.337	19.301	1.00 36.80
	1900	OH2	WAT	W	25	8.252	24.015	19.421	1.00 36.80
40	1901		WAT		26	-9.407	8.770	13.621	1.00 36.80
	1902	OH2	WAT	W	27	46.239	3.613	19.856	1.00 36.80
	1903	OH2	WAT	W	28	-1.747	5.460	-3.436	1.00 36.80
	1904	OH2	TAW	W	29	37.326	11.576	17.425	1.00 36.80

	1905	OH2	YAT	W	30		14.148	-10.191	16.523	1.00	36.80
	1906	OH2	TAW	W	31		15.836	20.107	8.725	1.00	36.80
	1907	ОН2	MAT	W	32		-4.798	11.641	14.018	1.00	36.80
	1908	OH2	WAT	W	33		-7.822	7.982	31.296	1.00	36.80
5	1909	ОН2	. WAT	W	34		3.598	15.873	33.954	1.00	33.31
	1910	ОН2	TAW :	W	35		10.074	21.605	27.336	1.00	33.31
	1911	ОН2	WAT	W	36		18.840	22.270	14.224	1.00	33.31
	1912	OH2	WAT	W	37		-1.792	24.266	11.374	1.00	33.31
	1913	OH2	WAT	W	38	,	-8.931	8.878	19.966	1.00	33.31
10	1914	OH2	WAT	M	39		-3.553	21.551	14.907	1.00	33.31
	1915	OH2	WAT	M	40		8.399	-0.175	13.515	1.00	33.31
	1916	OH2	WAT	W	41		-6.204	12.470	11.990	1.00	33.31
	1917	OH2	WAT	W	42		. 4.589	8.276	34.603	1.00	33.31
	1918	OH2	WAT	W	43		28.648	16.280	19.235	1.00	33.31
15	1919	OH2	WAT	W	44		18.590	15.236	-2.478	1.00	33.31
	1920	OH2	WAT	W	45		-9.057	0.909	19.891	1.00	33.31
	1921	OH2	TAW	W	46	,	-4.172	-4.775	22.498	1.00	33.31
	1922	OH2	TAW	W	47		2.411	6.885	32.413	1.00	33.31
	1923	OH2	WAT	W	48		12.792	13.554	-5.547	1.00	33.31
20	1924	OH2	WAT	W	49		-4.512	-6.634	11.993	1.00	33.31
	1925	OH2	WAT	W	50		-1.349	8.211	-3.909	1.00	33.31
	1926	OH2	WAT	W	51		13.234	14.853	39.074	1.00	33.31
	1927	OH2	WAT	W	52		37.819	4.036	7.107	1.00	33.31.
	.1928	. OH2	WAT	W	5.3		-3.499	3.773	29.867	1.00	33.31
25	1929	OH2	WAT	W	54		2.292	20.765	40.034	1.00	33.31
	1930		WAT		55		15.806	-0.857	-1.454	1.00	33.31
	1931		TAW		56		3.305	-4.239	15.620	1.00	36.80
	1876		TAW		1		3.683		28.746	1.00	36.80
20	1877		WAT		2		16.001	-0.936	41.994	1.00	36.80
30	1878		WAT		3		•	0.631			36.80
	1879				4			-3.880	47.608	1.00	36.80
	1880		WAT		5		15.507	-9.355	24.152	1.00	36.80
	1881		WAT		6			3.621		1.00	36.80
25	1882		TAW					-13.312	17.093	1.00	36.80
35	1883	OH2							47.826		36.80
	1884		WAT		9			-15.650	24.990	1.00	36.80
	1885		WAT		10			-23.017			36.80
	1886		WAT		11		•	-12.220			36.80
40	1887	OH2			12			-12.537			36.80
40	1888		WAT		13				25.171		36.80
	1889		WAT		14			-1.540			36.80
	1890		WAT		15			-15.036			36.80
	1891	OH2	WAT :	X	16		32.358	-3.652	9.291	1.00	36.80

```
1892 OH2 WAT X
                       17
                                22.480 -20.917
                                                22.300
                                                        1.00 36.80
      1893
            OH2 WAT X
                       18
                                26.786
                                        9.394 49.961
                                                        1.00 36.80
      1894
            OH2 WAT X
                       19
                                24.764 10.222
                                                26,384
                                                        1.00 36.80
            OH2 WAT X
      1895
                       '20
                                19.198
                                        ,6.611
                                                43.913
                                                        1.00 36.80
  5
      1896
            OH2 WAT X
                      21
                                26.159
                                        3.765
                                               33.066
                                                      1.00 36.80
      1897
                                4.678 -6.071
            OH2 WAT X
                       22
                                               57.076
                                                       1.00 36.80
      1898
            OH2 WAT X
                       23
                               21.861 -28.995
                                               44.438
                                                        1.00 36.80
      1899
            OH2 WAT X
                       24
                               27.866 -18.095 26.551
                                                        1.00 36.80
      1900
            OH2 WAT X
                       25
                               14.858 -24.079
                                               36.759 1.00 36.80
 10
      1901
            OH2 WAT X
                       26
                                4.325 -9.116
                                               52.350
                                                       1.00 36.80
      1902
            OH2 WAT X
                       27
                               43.966 -2.985
                                               12.943
                                                       1.00 36.80
      1903
            OH2 WAT X
                       28
                               20.854 -5.533 60.983
                                                       1.00 36.80
      1904
            OH2 WAT X
                       29
                               38.644 -11.092
                                               20.340
                                                       1.00 36.80
      1905
            OH2 WAT X
                       30 .
                               20.619 10.252
                                               35.552
                                                       1.00 36.80
 15
      1906
           OH2 WAT X
                       31
                               27.367 -19.948 40.456 1.00 36.80
      1907
           OH2 WAT X
                       32
                                7.746 -11.905
                                              49.162
                                                       1.00 36.80
      1908 OH2 WAT X
                      33
                               -5.421 -8.437 37.514
                                                       1.00 36.80
     1909
           OH2 WAT X
                       34
                                2.031 -16.137
                                               28.299
                                                       1.00 33.31
     1910
           OH2 WAT X
                       35
                               11.326 -21.697
                                               29.436
                                                       1.00 33.31
20
     1911
           OH2 WAT X
                       36
                               26.349 -22.099
                                               34.269
                                                       1.00 33.31
     1912
           OH2 WAT X
                       37
                               11.987 -24.451 49.302
                                                       1.00 33.31
     1913
           OH2 WAT X
                       38
                                0.761 -9.265
                                              47.080
                                                       1.00 33.31
     1914
           OH2 WAT X
                       39
                                8.361 -21.797 47.640
                                                       1.00 33.31
     1915 OH2 WAT X
                       40
                               18.174
                                       0.155
                                               41.426
                                                      1.00 33.31
25
     1916 OH2 WAT X
                       41
                                7.919 -12.744
                                              51.620
                                                      1.00 33.31
     1917
           OH2 WAT X
                       42
                                2.259 -8.529
                                               27.215
                                                       1.00 33.31
     1918
           OH2 WAT X
                       43
                             30.809 -15.968
                                               24.283
                                                       1.00 33.31
           OH2 WAT X
     1919
                      44
                               36.386 -14.940
                                               47.555
                                                       1.00 33.31
     1920
           OH2 WAT X
                      45
                               0.555 -1.299
                                               47.259
                                                       1.00 33.31
30
     1921 OH2 WAT X
                      46
                               2.656
                                       4.453
                                               42.213 1.00 33.31
     1922
          OH2 WAT X
                      47
                               1.885 -7.161
                                               30.291
                                                       1.00 33.31
     1923
           OH2 WAT X
                      48
                              33.715 -13.341
                                              53.569
                                                       1.00 33.31
     1924
           OH2 WAT X
                      49
                               8.875
                                       6.387
                                              50.669
                                                       1.00 33.31
     1925
           OH2 WAT X
                      50
                              21.512 -8.272
                                              61.092
                                                       1.00 33.31
35
     1926
          OH2 WAT X
                      51
                               6.385 -14.980
                                              18.308
                                                      1.00 33.31
     1927
          OH2 WAT X
                      52
                              45.290 -3.463
                                              28.162
                                                      1.00 33.31
    1928
          OH2 WAT X
                      53
                              -1.227 -4.138
                                              35.973
                                                      1.00 33.31
    1929
           OH2 WAT X
                      54
                              -2.672 -21.100
                                              24.317
                                                      1.00 33.31
    1930
          OH2 WAT X
                      55
                              33.258 1.090
                                              48.566
                                                      1.00 33.31
40
    1931
          OH2 WAT X
                      56
                              12.796
                                      4.108
                                              42.960
                                                      1.00 36.80
    END
```

PCT/US02/38715

Table IC
Atomic coordinates of UPPS in complex with IPP

	CR	YST1	5.9	. 42	28	118.1	68	175.	973	90.	00	90.	00 9	0.00
5	ATO	MC	RES	ID	JΕ		<u>X</u>		<u>y</u>		<u>z</u>		<u>0cc</u>	<u>B</u>
	1	СВ	GLN	A	18		7.9	46	25.13	18	75.	253	1.00	80.17
	2	CĢ	GLN	A	18		8.3	344	25.1	55	76.	710	1.00	83.70
	3	CD	GLN	A	18		7.1	.66	25.02	25	77.	641	1.00	85.97
	4	OE1	GLN	A	18		6.2	96	24.1	65	77.	449	1.00	88.60
10	5	NE2	GLN	Α	18		7.1	.31	25.86	69	78.	670	1.00	86.19
	6	С	GLN	A	18		8.8	55	24.34	42	73.	075	1.00	71.58
	7	0	GLN	A	18		7.6	97	24.07	74	72.	743	1.00	71.79
	8	N	GLN	A	18	*	9.5	69	26.52	28	74.0	025	1.00	72.89
	9	CA	GLN	A	18		9.1	57	25.12	28	74.3	330	1.00	72.72
15	10	N	VAL	Α	19	•	9.	929	23.9	964	72	.392	1.00	76.37
	11	CA	VAL	Α	19		9.	836	23.2	216	71	.156	1.00	74.76
	12	CB	VAL	Α	19		10.	081	24.1	L40	69	.983	1.00	77.30
	13	CG1			19		8.	898	25.0	79	69	.823	1.00	76.99
20	14		VAL		19		11.	372	24.9	15	70.	.222	1.00	74.13
20	15	С	VAL		19		10.	822	22.0		71.	.076	1.00	72.83
	16	0	VAL		19		11.	780	21.9	82	71.	.841	1.00	73.33
	17	N	PRO		20		10.		21.1		70.	.132		45.38
	18	CD	PRO		20			422	21.1		69.	.233	1.00	63.68
25	19	CA	PRO		20		11.		19.9			912	1.00	42.31
25	20	CB	PRO		20		10.		19.0			022	1.00	
	21	CG	PRO		20			821	20.1	.01		208		63.80
	22	С	PRO		20		12.		20.2			270		39.14
	23	0	PRO		20		12.		20.8			195	1.00	36.95
20	24	N	ALA		21		13.		19.8			932	1.00	
30	25	CA	ALA		21		15.		20.1			408		43.37
	26	CB	ALA		21		16.		19.6			409		19.22
	27	C	ALA		21		15.		19.4			067	1.00	
	28	0	ALA		21		16.		19.8			238		41.42
35 .	29	N CZ	HIS		22		14.		18.2			860		50.77
JJ	30	CA	HIS		22		14.8		17.5			631		49.24
	31	CB	HIS HIS		22		15.		16.3			896		40.18
	32	CG			22		16.		15.5			676		38.94
	33		HIS		22		15.4		15.3			509		37.84
40	34		HIS		22		17.2		14.7			570		40.51
+0	35 36		HIS		22		17.3		14.2			388		40.05
	36 37		HIS		22		16.2		14.5			725		40.19
	37 30	С	HIS		22		13.5		17.0			038		49.35
	38	0	HIS	A	22	,	12.9	129	16.2		66.	630	1.00	49.93
									319	7				

	39	N	ΙL	E A	23		13.229	17.556	64.865	1.00	50.60
	40	CA	ΙL	ΕA	23		12.012	17.127	64.185	1.00	52.08
	41	СВ	IL	E A	23		11.116	18.303	63.770	1.00	52.30
	42	CG	2 IL	ΕA	23		9.907	17.785	63.017	1.00	49.04
5	43	CG:	l IL	ΕA	23		10.606	19.039	64.996	1.00	52.99
	44	CD:	LIL	ΕA	23		9.575	18.258	65.745	1.00	55.11
	45	С	IL	E A	23	,	12.372	16.371	62.914	1.00	53.34
	46	0	IL	E A	23		13.278	16.763	62.186	1.00	52.81
	47	N	GL	ΥA	24		11.664	15.280	62.655	1.00	55.59
10	48	CA	GL.	Y A	24		11.916	14.510	61.454	1.00	55.68
	49	С	GL.	ΥA	24		10.636	14.558	60.652	1.00	57.28
	50	0	GL.	Y A	24		9.561	14.279	61.188	1.00	58.15
	51	N	IL	ΕΑ	25		10.723	14.925	59.379	1.00	60.87
	52	CA	IL	ΞΑ	25		9.518	14.997	58.574	1.00	60.55
15	53	CB	ILI	ΞΑ	25	•	9.274	16.407	58.016	1.00	44.36
	54	CG2	LL	E A	25		7.783	16.649	57.880	1.00	43.36
	55	CG1	. IL	ΞΑ	25		9.863	17.464	58.946	1.00	43.88
	56	CD1			25		9.805	18.870	58,385	1.00	40.84
	57	С	ILF		25	•	9.628	14.080	57.388	1.00	61.16
20	58	0	ILE		25		10.688	13.955°	56.781	1.00	61.90
	59	N	ILE		26	. •	8.526	13.430	57.062	1.00	50.76
	60	CA	ILE		26		8.491	12.557	55.912		51.38
	61	CB			- 26		7.771	11.250	56.229	A 6.74 97	39.40
25	62	CG2			26		7.530	10.469	54.944		36.96
23	63	CG1			26		8.590	10.437	57.231	*.	38.89
	64 65	CD1 C			26		7.963	9.106	57.576		36.95
	66	0	ILE		26		7.669	13.332	54.905		52.89
	67	N	ILE MET		26 27		6.455	13.472	55.089		52.47
30	68	CA	MET		27		8.333 7.696	13.838	53.861 52.808		56.05
	69	СВ	MET		27		8.733	15.596			57.51
	70	CG	MET		27		9.433	16.489	52.181 53.193		43.28
	71	SD	MET		27		10.718	17.550	52.514		33.89
	72	CE	MET		27		12.040	16.489	52.414		32.98
35	73	С	MET		27		6.998	13.821	51.708		61.12
	74	0	MET		27		7.577	13.539	50.653		61.44
	75	N	ASP		28		5.738	13.469	51.968		78.26
	76	CA	ASP		28		4.906	12.680	51.056		81.87
	77	СВ	ASP		28		4.483	11.376	51.743	1.001	
40	78	CG	ASP		28		3.741	10.431	50.809	1.001	
	79	OD1			28		4.298	10.095	49.740	1.001	
	80	OD2			28		2.609	10.016	51.146	1.001	
	81	С	ASP		28		3.655	13.455	50.635	1.00	

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82
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               ASP A
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                                        14.385 51.319
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          ·N
               GLY A
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      84
          CA
               GLY A
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10
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              GLY A
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           CG
               ARG A
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                                        12.357
                                                 46.121
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               ARG A
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25
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                                        13.288
                                                 50.746
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           С
               ARG A
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           CG
               TRP A
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                                                         1.00 87.76
           CD2 TRP A
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               ALA A
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                                        18.209
                                                 43.546
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```

	105	~~	~ ~ ~	•	2.4		0 00.0	10 000	40 010	1 00100 60
•	125	CA			34		0.086			1.00103.60
	126	CB	ALA		34		1.553	19.001	41.778	1.00 43.07
	127	C	ALA		34		-0.692	18.001	41.163	1.00104.15
5	128	_	ALA		34		-0.767	18.388	39.998	1.00104.13
5	129	N	LYS		35		-1.278	16.884		1.00102.73
	130	CA	LYS		35		-2.070	16.049	40.689	1.00104.36
	131	СВ	LYS		35		-2.305	14.670	41.327	1.00103.46
	132	CG	LYS		35		-2.952	13.616	40.416	1.00103.78
	133	CD	LYS		35		-4.481	13.720	40.345	1.00104.86
. 10	134	CE	LYS		35		-5.060	12.605	39.472	1.00104.77
	135	ΝZ	LYS		35		-6.547	12.587	39.430	1.00103.24
	136	С	LYS	A	35		-3.409	16.750	40.409	1.00104.89
	137	0	LYS	A	35	•	-3.633	17.247	39.303	1.00104.89
	138	N	LYS	A	36		-4.283	16.799	41.415	1.00108.67
15	139	CA	ĻYS	A	36		-5.596	17.433	41.288	1.00108.81
	140	CB	LYS	A	36		-6.275	17.496	42.656	1.00116.28
	141	CG	LYS	A	36		-7.584	18.276	42.663	1.00116.03
	142	CD	LYS	A	36		-7.654	19.234	43.851	1.00115.08
	143	CE	LYS	A	36		-6.594	20.332	43.760	1.00114.82
20	144	NZ	LYS	A	36		-6.626	21.277	44.921	1.00113.37
	145	С	LYS	A	36		-5.547	18.844	40.694	1.00108.73
	146	0	LYS	A	36		-6.529	19.321	40.115	1.00108.16
	147	N	ARG	A	37		-4.407	19.510	40.850	1.00111,25
	148	CA	ARG	A	37		-4.226	20.863	40.334	1.00111.49
25	149	СВ	ARG	A	37		-2.984	21.503	40.954	1.00 99.74
	150	CG	ARG	A	37		-3.031	21.668	42.457	1.00100.08
	151	CD	ARG	A	37		-4.044	22.718	42.877	1.00100.41
	152	NE	ARG	A	37		-3.537	23.542	43.974	1.00100.65
	153	CZ	ARG	A	37		-3.282	23.099	45.203	1.00100.42
30	154	NH1	ARG	A	37		-3.489	21.825	45.522	1.00100.28
	155	NH2	ARG	A	37		-2.800	23.938	46.110	1.00100.50
	156	С	ARG	A	37		-4.071	20.885	38.817	1.00111.43
	157	0	ARG	A	37		-3.974	21.957	38.222	1.00111.99
	158	N	MET	A	38		-4.049	19.707	38.198	1.00 98.41
35	159	CA	MET	A	38		-3.875	19.595	36.749	1.00 97.99
	160	СВ	MET .	A	38	•	-4.941	20.407	36.004	1.00115.32
	161	CG	MET .	A	38	-	-6.343	19.822	36.074	1.00116.27
	162	SD	MET .	A	38		-6.439	18.168	35.357	1.00117.85
	163	CE	MET .	A	38		-6.633	18.546	33.608	1.00116.66
40	164	С	MET I		38		-2.483	20.107	36.393	1.00 97.09
	165	0	MET 2		38		-2.304	20.916	35.478	1.00 96.60
	166	N	GLN 2		39		-1.499	19.623	37.137	1.00 91.07
	167	CA	GLN Z		39		-0.117	20.021	36.928	1.00 90.66
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	214		GLY				5.981	20.042		1.00 81.72
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	218	CG	HIS	A	45		8.646	16.023	43.467	1.00 89.70
	219	CD2	HIS	A	45		7.864	15.119	42.828	1.00 90.25
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	222	NE2	HIS	A	45		7.683	14.059	43.684	1.00 90.18
	223	С	HIS	A	45		8.916	19.882	43.505	1.00 91.27
	224	0	HIS	A	45		9.828	20.149	44.296	1.00 91.42
15	225	N	LYS	, A	46	•	8.487	20.734	42.577	1.00 82.42
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	227	CB	LYS	A	46		8.683	22.710	41.114	1.00 97.17
	228	CG	LYS		46		9.491	22.162	39.947	1.00 99.47
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20	230	CE	LYS		46		10.094	22.419	37.536	1.00 99.93
	231	NZ	LYS		46		9.782	23.075	36.241	1.00100.68
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	233	Ö	LYS		46		8.927	23.727	44.207	1.00 80.53
25	235	N CA	ALA		47		7.085	22.485	43.813	
23	235	CB	ALA ALA		47 47	1	6.276	23.094	44.858	
	237	С	ALA		47		4.819	23.105	44.452	1.00 69.13
	238	0	ALA		47		5.505	22.241 21.722	46.094 46.665	1.00 75.37
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30	240	CA	GLY		48		8.044			1.00 73.42
	241	С	GLY		48		9.323			1.00 74.36
	242	0	GLY	A	48		9.384	21.985	49.491	1.00 74.58
	243	N	MET	A	49		10.355		47.458	1.00 81.06
	244	CA	MET	A	49		11.628	22.480	47.963	1.00 81.70
35	245	CB	MET	A	49		12.641	22.627	46.825	1.00 87.38
	246	CG	MET	A	49		13.136	21.307	46.243	1.00 87.33
	247	SD	MET	A	49		14.010	21.505	44.663	1.00 87.62
	248	CE	MET	A	49		12.610	21.420	43.554	1.00 85.01
	249	.C	MET	A	49		11.320	23.833	48.586	1.00 81.21
40	250	0	MET	A	49		11.946	24.240	49.564	1.00 81.58
	251	N	GLU .	A	50		10.337	24.517	48.007	1.00 77.92
	252	CA	GLU .	A	50		9.900	25.810	48.506	1.00 77.34
	253	CB	GLU .	A	50		8.822	26.402	47.588	1.00 95.37

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	254	CG	GL	JA	50		9.050	27.860	47.157	1.00	95.61
	255	CD	GL	JA	50	,	9.139	28.834	48.326	1.00	96.16
	256	OE:	1 GL	JA	50		8.198	28.884	49.148	1.00	95.48
	257	OE:	2 GL	JA	50		10.154	29.556	48.417	1.00	96.34
5	258	С	GL	JÁ	50		9.306	25.500	49.873	1.00	76.40
	259	0	GL	JA	50		9.684	26.094	50.883	1.00	76.44
	260	N	ALA	A A	51		8.377	24.551	49.896	1.00	70.94
	261	CA	ALA	AA	51	,	7.741	24.135	51.142	1.00	69.92
	262	CB	ALA	AA	51		6.856	22.914	50.889	1.00	99.69
10	263	С	ALA	ÀÀ	51		8.798	23.817	52.207	1.00	68.95
	264	0	ALA	A	51		8.601	24.073	53.393	1.00	68.42
	265	N	LEU	JA	52		9.914	23.242	51.775	1.00	66.05
	266	CA	LEU	JA	52		10.998	22.922	52.689	1.00	65.82
	267	СВ	LEU	A	52		12.066	22.062	51.993	1.00	68.86
15	268	CG	LEU	A	52		13.451	21.922	52.648	1.00	67.64
	269	CD1	LEU	Α	52		13.322	21.671	54.148	1.00	67.79
	270	CD2	LEU	Α	52		14.210	20.788	51.977	1.00	65.11
	271	С	LEU	Α	52		11.601	24.242	53.116	1.00	65.19
	272	0	LEU	Α	52 .		11.896	24.446	54.288	1.00	64.48
20	273	N	GLN	A	53		11.759	25.132	52.140	1.00	76.33
	274	CA	GLN	A	53		12.325	26.459	52.347	1.00	75.19
	275	CB	GLN	A	53		12.367	27.216	51.022	1.00	69.00
,	276	CG	GLN	Ą	53		13.340	28.356	51.018	1.00	68.46
*	277	CD	GLN	A	53		14.740	27.863	51.257	1.00	68.74
25	278、	OE1	GLN	Α	53		15.006	27.198	52.256	1.00	69.27
,	279	NE2	GLN	A	53		15.647	28.175	50.339	1.00	67.93
	280	С	GLN	A	53		11.519	27.265	53.355	1.00	74.92
	281	0	GLN	A	53		12.068	28.045	54.126	1.00	74.08
20	282	N	THR	A	54		10.209	27.081	53.334	1.00	84.09
30	283	CA	THR	A	54		9.340	27.782	54.258	1.00	84.86
	284	CB	THR	A	54		7.870	27.659	53.820	1.00	67.41
	285	OG1	THR	A	54		7.669	28.444	52.639	1.00	68.01
	286		THR		54		6.922	28.124	54.928	1.00	66.49
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35	288	0	THR	А	54		9.546	27.970	56.638	1.00	86.21
	289	N	VAL	A	55		9.579	25.884	55.764	1.00	69.54
	290	CA	VAL	A	55		9.710	25.189	57.051	1.00	67.41
	291	CB	VAL		55		9.164	23.745	56.973	1.00	69.10
40	292		VAL		55		9.287	23.091	58.325	1.00	68.82
40	293		VAL		55		7.705	23.744	56.534	1.00	68.80
	294	С	VAL		55		11.128	25.141	57.625	1.00	67.02
	295	0	VAL	A	55		11.327	25.472	58.791	1.00	67.32
	296	N	THR	A	56		12.111	24.722	56.832	1.00	58.40

	297	CA	тн	R A	56	13.480	24.689	57.341	1.00 59.09
	298	СВ	TH	R A	56	14.520	24.231	56.257	1.00 61.50
	299	OG	1 TH	R A	56	15.859	24.425	56.750	1.00 60.24
	300	CG	2 TH	R A	56	14.351	25.021	54.981	1.00 64.31
5	301	С	TH:	R A	56	13.827	26.103	57.802	1.00 59.69
	302	Ο.	TH:	R A	56	14.827	26.327	58.500	1.00 60.34
	303	N	LY	s A	57	12.973	27.046	57.405	1.00 74.50
	304	CA	LY	S A	. 57	13.118	28.466	57.726	1.00 74.27
	305	СВ	LY	S A	. 57	12.374	29.300	56.672	1.00 59.08
10	306	CG	LYS	SA	. 57	12.783	30.751	56.603	1.00 59.25
	307	CD	LYS	S A	. 57	12.913	31.221	55.158	1.00 60.46
	308	CE	LYS	s A	57	11.557	31.349	54.476	1.00 62.59
	309	NZ	LYS	5 A	57	11.681	31.790	53.056	1.00 60.91
•	310	С	LYS	5 A	57	12.520	28.701	59.101	1.00 74.12
15	311	0	LYS	S A	57	13.228	29.020	60.062	1.00 74.74
	312	N	ALA	A	58	11.204	28.526	59.171	1.00 63.23
	313	CA	ALF	A A	58	10.456	28.684	60.405	1.00 63.11
	314	CB	ALA	A	58	9.019	28.284	60.182	1.00 34.72
	315	·C	ALA	A	58	11.089	27.785	61.452	1.00 63.84
20	316	0	ALA	A	58	11.256	28.172	62.612	1.00 63.83
	317	N	ALA	A	59	11.434	26.575	61.028	1.00 82.06
	318	CA	ALA	A	59	12.068	25.615	61.907	1.00 81.68
	. 319	СВ	ALA	A	59	12.589	24.453	61.100	1.00 82.06
	320	С	ALA	Α	59	13.219	26.302	62.635	1.00 82.43
25	321	0	ALA	Α.	59	13.247	26.358	63.864	1.00 82.77
	322	N	ASN	Α	60	14.160	26.837	61.865	1.00 89.28
	323	CA	ASN	A	60	15.319	27.521	62.425	1.00 89.34
	324	CB	ASN		60	16.229	28.003	61.292	1.00 67.34
20	325	CG	ASN	A	60	17.591	28.441	61.788	1.00 67.19
30	326	OD1			60	18.176	27.796	62.651	1.00 67.36
	327		ASN		60	18.113	29.530	61.232	1.00 67.97
	328	С	ASN		60	14.888	28.702	63.289	1.00 89.22
	329	0	ASN	Α	60	15.512	29.008	64.305	1.00 89.44
	330	N	LYS	A	61	13.805	29.352	62.880	1.00 65.39
35	331	CA	LYS	A	61	13.277	30.507	63.597	1.00 65.03
	332	CB	LYS	A	61	12.132	31.127	62.786	1.00 97.09
	333	CG	LYS	A	61	11.459	32.356	63.412	1.00 98.41
	334	CD	LYS	A	61	10.527	33.060	62.407	1.00 98.42
40	335	CE	LYS		61	9.436	32.130	61.884	1.00 98.05
40	336	NZ	LYS		61	8.681	32.724	60.750	1.00 97.33
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	338	0	LYS		61	13.407	30.563	65.993	1.00 61.87
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	384	CE	з тн	R F	4 68	15.928	3 14.150	59.936	
	385	00	51 TH	R	4 68	16.994	14.427	60.849	1.00 47.66
•	386	ce	32 TH	R A	68	16.444	13.207	58.887	1.00 50.16
5	387	C	TH	R A	4 68	14.299	15.224	58.365	1.00 46.51
	388	0	. TH	R A	68	13.194	14.868	58.792	1.00 44.30
•	389	N	VA	L A	69	14.560	15.478	57.086	1.00 41.74
	390	CA	. VA	L A	69	13.575	15.358	56.014	1.00 43.69
	391	CB	VA	LΑ	69	13.657	16.564	55.062	1.00 58.55
10	392	CG	1 VA	LΑ	69	13.219	17.831	55.789	1.00 57.65
	393		2 VA:	L A	. 69	15.089	16.705	54.524	1.00 58.16
	394		VA	LΑ	. 69	13.773	14.097	55.190	1.00 44.57
	395		VA:	LΑ	69	14.863	13.837	54.673	1.00 43.05
4.5	396	N	TYI	R A	70	12.707	13.318	55.068	1.00 59.78
15	397	CA	TYI	R A	70	12.760	12.075	54.325	1.00 62.67
	398		TY	R A	70	11.929	11.009	55.031	1.00 52.64
	399	CG		R A		12.143	9.625	54.494	1.00 49.53
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	403		2 TYF		70	11.424	7.329	54.260	1.00 48.99
	404	CZ	TYR		70	12.587	7.041	53.557	1.00 48.59
	405 406	OH C	TYR		70	12.816	5.770	53.100	1.00 48.72
25	407	0	TYR TYR		70 70	12.208	12.353	52.954	1.00 66.44
- 9,	408	N	ALA		71	11.023	12.625	52.796	1.00 65.91
	409	CA	ALA		71	13.077 12.692	12.270	51.959	1.00 68.56
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	411	С	ALA		71	12.111	13.176 11.423	49.878	1.00 72.73
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	413	N	PHE		72	10.796	11.197	49.859	1.00 78.80
	414	CA	PHE		72	10.088	10.161	49.080	1.00 89.46
	415	СВ	PHE		72	11.012	8.973	48.765	1.00 03.40
	416	CG	PHE	Α	72	10.397	7.944	47.849	1.00144.03
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	418	CD2	PHE	A	72	10.457	6.588	48.163	1.00144.94
	419	CE1	PHE	A	72	9.204	7.378	45.815	1.00146.82
	420	CE2	PHE	A	72	9.897	5.628	47.314	1.00146.70
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5	430	N	THE	A	74	•	6.642	6.983	48.613	1.00161.50
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	432	СВ	THE	A	74	,	4.495	5.764	48.297	1.00143.68
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,	434	CG2	THR	A	74	,	3.518	5.267	47.238	1.00143.83
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40	465		TRP		77		0.169	11.961	42.099	1.00169.90
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	46	9 C	А Т	HR :	A 78		3.248	3.70	0 39.51	9 1.00114.21
	47	0 C	в т	HR Z	A 78		2.400	3.26	8 38.30	3 1.00109.37
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5	47	3 , C	T.	HR, A	A 78		4.681	3.89	39.05	1 1.00113.51
	47	4 0	T.	HR A	A 78	•	5.342	4.872	2 39.388	•
	47	5 N	A	RG A	A 79		5.142	2.922	38.26	3 1.00125.73
	47	6 C2	A A	RG 1	A 79		6.480	2.924	37.702	2 1.00124.36
	47	7 CI	a Al	RG I	A 79	•	6.630	4.068	36.696	1.00100.13
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	479	e CI	AI	RG P	A 79		4.510	3.914	35.335	1.00 99.41
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	481	L CZ	A	RG A	79		4.263	4.207	32.894	1.00 99.40
	482	NH.	11 AF	RG A	79		5.151	5.196	32.901	1.00 98.32
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	1207	CG	ASN A 170	36.777	-7.908	73.288	1.00 95.03
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10	1295	CG	TYR	A	182	29.496	1.931	64.458	1.00	48.01
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	1306	CB	LEU	A	183	23.218	5.203	63.490	1.00	.39.84
	1307	CG	ΓEÑ	Α	183	22.754	3.944	64.233	1.00	36.79
	1308	CD1	LEU	Ą	183	21.519	4.267	65.018	1.00	36.60
	1309	CD2	LEU	Α	183	22.457	2.828	63.260	1.00	36.31
25	1310	С	LEU	A	183	24.753	6.308	61.841	1.00	48.51
	1311	0	LEU	A	183	25.705	7.019	62.099	1.00	50.48
	1312	N	PHE	A	184	23.912	6.578	60.853	1.00	48.19
	1313	CA	PHE	A	184	24.091	7.747	59.994	1.00	49.49
	1314	CB	PHE	A	184	23.081	7.725	58.849		44.20
30	1315	CG	PHE	A	184	23.347	6.671	57.820	1.00	44.57
	1316	CD1	PHE	A	184	22.477				44.44
	1317		PHE			24.448	5.837			44.74
		CE1	PHE	A		22.696				44.26
			PHE	A		24.676				43.37
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		CA	THR				10.308	62.487		50.50
40	1325	CB	THR				10.113	63.422		44.57
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	1328	С	THR	Α	185	24.050	10.649	63.370	1.00	54.78

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	1331	CA	GLN	A	186	26.291	9.988	64.115	1.00	60.77
	1332	СВ	GLN	Α	186	27.387	9.029	63.654	1.00	92.96
5	1333	CG	GLN	A	186	27.942	9.355	62.282	1.00	96.28
	1334	CD	GLN	A	186	29.106	8.469	61.894	1.00	98.93
	1335	OE1	. GLN	A	186	28.952	7.260	61.722	1.00	100.11
	1336	NE2	GLN	.A	186	30.284	9.068	61.756	1.00	100.05
	1337	С	GLN	A	186	26.816	11.404	64.002	1.00	63.76
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•	1341	CB	HIS	A	187	27.415	13.451	60.957	1.00	75.76
	1342	CG	HIS	A	187	28.288	12.465	60.246	1.00	76.39
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	1344	ND1	HIS	A	187	29.636	12.341	60.507	1.00	76.18
	1345	CE1	HIS	A	187	30.146	11.394	59.738	1.00	77.18
	1346	NE2	HIS	A	187	29.178	10.899	58.988	1.00	76.82
	1347	С	HIS	A	187	26.502	14.333	63.091	1.00	65.00
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	1349	N	LEU	A	188	26.201	14.182	64.374	1.00	63.51
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	1351	CB	LEU	A	188	23.888	14.904	64.818	1.00	67.36
	1352	CG	LEU	A	188	23.177	15.455	63.567	1.00	68.27
25	1353	CD1	LEU	A	188	23.581	14.720	62.288	1.00	67.48
	1354	CD2	LEU	A	188	21.674	15.303	63.785	1.00	68.32
	1355	С	LEU	A	188	25.649	15.042	66.607	1.00	66.30
	1356	0	LEU	A	188	26.180	14.047	67.097	1.00	66.36
	1357	N	PRO	A	189	25.279	16.078	67.363	1.001	.00.45
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40	1368	CD	LYS	A	190	27.938	10.688	72.165	1.00	96.56
	1369	CE	LYS	A	190	29.027	9.877	71.460	1.00	96.04
	1370	NZ	LYS			29.800	9.013	72.413	1.00	96.75
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	1374	CA	ASP	A	191	21.975	14.773	72.459	1.00 83.52
•	1375	СВ	ASP	A	191	22.312	15.829	73.526	1.00118.93
5	1376	CG	ASP	A	191	23.039	17.042	72.955	1.00121.92
	1377	OD1	ASP	Α	191	24.050	16.861	72.242	1.00122.89
	1378	OD2	ASP	A	191	22.608	18.182	73.229	1.00122.16
	1379	С	ASP	A	191	20.831	15.253	71.584	1.00 80.20
	1380	0	ASP	A	191	19.785	15.671	72.084	1.00 79.39
10	1381	N	LEU	A	192	21.040	15.182	70.273	1.00 72.77
	1382	CA	LEU	A	192	20.038	15.597	69.294	1.00 69.38
	1383	СВ	LEU	A	192	20.429	16.939	68.684	1.00 72.72
	1384	CG	LEU	A	192	20.070	18.160	69.520	1.00 72.64
	1385	CD1	LEU	A	192	21.228	19.131	69.548	1.00 74.95
15	1386	CD2	LEU	A	192	18.831	18.805	68.945	1.00 72.23
	1387	С	LEU	A	192	19.898	14.553	68.191	1.00 66.49
	1388	0	LEU	A	192	19.062	14.686	67.299	1.00 65.42
	1389	N	ARG	A	193	20.731	13.518	68.267	1.00 50.93
Y	1390	CA	ARG	A	193	20.728	12.428	67.297	1.00 46.98
20	1391	СВ	ARG	A	193	21.658	11.312	67.794	1.00 49.52
	1392	CG	ARG	A	193	23.152	11.689	67.813	1.00 49.10
	1393	CD	ARG	A	193	24.032	10.612	68.489	1.00 47.28
	1394	NE	ARG			25.452	10.736	68.150	1.00 47.28
	1395	CZ	ARG	A	193	26.392	9.851	68.479	1.00 48.04
25	1396	NH1	ARG	A	193	26.082	8.759		1.00 46.77
	1397	NH2	ARG	A	193	27.649	10.048	68.096	1.00 50.46
	1398	С	ARG	A	193	19.316	11.877	67.032	1.00 44.00
	1399	0	ARG			18.916	11.683		1.00 42.42
20	1400		ASP			18.556		68.094	1.00 36.34
30	1401	CA	ASP			17.200	11.124	67.945	1.00 33.93
	1402					•	10.204		1.00 36.54
	1403	CG	ASP			17.866			1.00 34.55
	1404		ASP				•		1.00 34.00
25	1405		ASP			17.833			1.00 33.59
35	1406					16.093			1.00 32.88
	1407		ASP			15.891			1.00 31.68
	1408	N	PRO			15.341			1.00 34.77
	1409	CD	PRO			15.303			1.00 55.68
40	1410	CA	PRO			14.260			1.00 34.35
40	1411	CB	PRO			13.481		65.388	1.00 55.61
	1412	CG	PRO			14.515			1.00 56.45
	1413	C			195				1.00 34.92
	1414	0	PRO	A	195	13.217	12.067	68.404	1.00 35.19

	1415	N	ASP	Ā	196	12.916	14.277	68.226	1.00	38.18
	1416	CA	ASP	A	196	12.043	14.355	69.394	1.00	39.88
	1417	СВ	ASP	A	196	12.166	15.717	70.073	1.00	55.77
	1418	CG	ASP	Α	196	13.510	15.921	70.733	1.00	59.88
5	1419	OD1	ASP	Α	196	13.796	17.056	71.157	1.00	61.23
	1420	OD2	ASP	A	196	14.282	14.951	70.842	1.00	60.04
	1421	С	ASP	A	196	10.642	14.204	68.837	1.00	40.38
	1422	0	ASP	Α	196	9.694	13.901	69,555	1.00	40.86
	1423	N	LEU	A	197	10.529	14.414	67.528	1.00	58.18
10	1424	CA	LEU	A	197·	9.251	14.329	66.847	1.00	59.97
	1425	СВ	LEU	A	197	8.507	15.638	67.063	1.00	39.96
	1426	CG	LEU	A	197	7.114	15.766	66.476	1.00	38.32
	1427	CD1	LEU	A	197	6.247	14.726	67.120	1.00	38.54
	1428	CD2	LEU	A	197	6.561	17.156	66.733	1.00	38.84
15	1429	С	LEU.	Α	197	9.378	14.031	65.346	1.00	61.27
	1430	0	LEŲ	A	197	10.228	14.581	64.654	1.00	63.27
	1431	N	ILE	Α	198	8.513	13.152	64.859	1.00	51.40
	1432	CA	ILE	Α	198	8.478	12.748	63.456	1:00	51.63
	1433	СВ	ILE	A	198	8.564	11.212	63.339	1.00	32.05
20	1434	CG2	ILE	Α	198	8.183	10.775	61.968	1.00	29.63
•	1435	CG1	ILE	A	198	9.982	10.743	63.666	1.00	31.32
	1436	CD1	ILE	Α	198	10.132	9.251	63.781	1.00	24.89
	1437	С	IĻĒ	A	198	7.150	13.219	62.870	1.00	54.08
	1438	0	ILE	Α	198	6.130	13.140	63.545	1.00	55.97
25	1439	Ŋ	ILE	A	199	7.149	13.709	61.629	1.00	55.58
	1440	CA	ILE	A	199	5.903	14.182	61.011	1.00	57.03
	1441	СВ	ILE	Α	199	5.928	15.712	60.782	1.00	61.40
	1442	CG2	ILE	Α	199	4.650	16.145	60.110	1.00	61.59
	1443	CG1	ILE	A	199	6.074	16.447	62.115	1.00	60.67
30	1444	CD1	ILE	A	199	6.203	17.943	61.985	1.00	57.19
	1445	С	ILE	A	199	5.585	13.509	59.674	1.00	58.15
	1446	0	ILE	A	199	6.399	13.520	58.748	1.00	59.57
	1447	N	ARG	A	200	4.394	12.925	59.586	1.00	40.62
	1448	CA	ARG	Α	200	3.949	12.251	58.369	1.00	41.42
35	1449	СВ	ARG	Α	200	3.544	10.795	58.658	1.00	57.13
	1450	CG	ARG	Α	200	3.372	9.936	57.402	1.00	54.89
	1451	CD	ARG	A	200	4.638	10.052	56.544	1.00	53.92
	1452	NE	ARG	A	200	4.596	9.341	55.268	1.00	52.83
	1453	CZ	ARG	Α	200	4.486	8.024	55.138	1.00	51.74
40	1454	NH1	ARG	A	200	4.398	7.247	56.212	1.00	52.92
	1455	NH2	ARG	A		4.487		53.928	1.00	50.95
	1456	С	ARG	A	200	2.749	12.986	57.804	1.00	43.70
	1457	0	ARG	A	200	1.723	13.129	58.477	1.00	42.74

	1458	N	THR	A	201	2.877	13.448	56.565	1.00	71.25
	1459	CA	THR	Α	201	1.798	14.174	55.908	1.00	74.12
	1460	СВ	THR	A	201	2.360	15.272	55.001	1.00	73.23
	1461	OG1	THR	A	201	2.913	14.673	53.828	1.00	76.28
5	1462	CG2	THR	Α	201	3.459	16.038	55.711	1.00	74.06
	1463	С	THR	Α	201	0.958	13.224	55.049	1.00	76.46
	1464	o	THR	A	201	1.174	12.011	55.048	1.00	78.25
	1465	N	SER	A	202	-0.007	13.784	54.328	1.00	55.00
	1466	CA	SER	A	202	-0.872	13.006	53.448	1.00	54.41
10	1467	СВ	SER	A	202	-0.103	12.603	52.196	1.00	53.35
	1468	OG	SER	A	202	-0.890	11.747	51.391	1.00	52.76
	1469	C	SER	A	202	-1.486	11.762	54.074	1.00	54.42
	1470	0	SER	A	202	-1.379	10.675	53.522	1.00	54.50
	1471	N	GLY	Α	203	-2.131	11.934	55.224	1.00	69.79
15	1472	CA	GLY	A	203	-2.782	10.835	55.918	1.00	70.25
	1473	С	GLY	Α	203	-2.218	9.446	55.678	1.00	71.00
	1474	0	GLY	A	203	-2.812	8.639	54.968	1.00	71.94
•	1475	N	GLU	A	204	-1.069	9.160	56.275	1.00	65.14
	1476	CA	GLU	A	204	-0.430	7.863	56.133	1.00	64.58
20	1477	СВ	GLU	A	204	0.783	7.975	55.207	1.00	89.40
	1478	CG	GLU	A	204	0.451	8.231	53.750	1.00	92.38
	1479	CD	GLU	A	204	0.034	6.970	53.018	1.00	94.85
	1480	OE1	GLU	A	204	-0.825	6.234	53.549	1.00	94.30
	1481	OE2	GLU	A	204	0.561	6.717	51.910	1.00	96.15
25	1482	C	GLU	A	204	0.025	7.430	57.516	1.00	63.86
	1483	0	GLU	A	204	0.831	8.120	58.146	1.00	64.30
	1484	N	LEU	A	205	-0.485	6.300	57.998	1.00	77.27
	1485	CA	LEU	A	205	-0.083	5.810	59.312	1.00	75.81
	1486	CB	LEU	A	205	-1.307	5.355	60.110	1.00	73.73
30	1487	CG	LEU	A	205	-2.419	6.400	60.268	1.00	73.58
	1488	CD1	LEU	A	205	-3.189	6.111	61.540	1.00	72.43
	1489	CD2	LEU	A	205	-1.840	7.801	60.327	1.00	73.40
	1490	С	LEU	A	205	0.961	4.690	59.233	1.00	74.05
	1491	0	LEU	A	205	0.782	3.609	59.797	1.00	73.90
35	1492	N	ARG	A	206	2.046	4.978	58.516	1.00	44.09
	1493	CA	ARG	A	206	3.179	4.081	58.336	1.00	43.58
	1494	CB	ARG	A	206	3.292	3.601	56.888	1.00	79.95
	1495	CG	ARG	A	206		2.805		1.00	82.38
	1496	CD	ARG	A	206		2.233			86.62
40	1497	NE	ARG	A	206	1.323		54.148		90.07
	1498	CZ			206			53.615		91.34
	1499	NH1	ARG	Α	206	0.973			1.00	90.96
	1500	NH2	ARG	A	206	-0.458	2.772	52.879	1.00	92.02

	1501	С	ARG	A 206	4.452	4.871	58.653	1.00 42.29
	1502	0	ARG	A 206	4.483	6.100	58.531	1.00 40.58
	1503	N	LEU	A 207	5.516	4.176	59.042	1.00 70.66
	1504	CA	LEU	A 207	6.755	4.889	59.327	1.00 68.57
5	1505	СВ	LEU	A 207	7.466	4.298	60.552	1.00 67.93
	1506	CG	LEU	A 207	8.184	5.399	61.344	1.00 69.26
	1507	. CD	1 LEU	A 207	7.131	6.282	61.992	1.00 67.83
	1508	CD	2 LEU.	A 207	9.114	4.820	62.390	1.00 69.87
	1509	С	LEU	A 207	7.683	4.883	58.100	1.00 66.21
. 10	1510	0	LEU	A 207	8.649	5.645	58.031	1.00 66.27
	1511	N	SER	A 208	7.384	4.017	57.138	1.00 48.52
	1512	CA	SER	A 208	8.152	3.937	55.895	1.00 44.95
	1513	СВ	SER	A 208	7.897	5.193	55.061	1.00 49.44
	1514	OG	SER .	A 208	6.505	5.438	54.934	1.00 53.00
15	1515	С	SER .	A 208	9.655	3.741	56.049	1.00 42.59
	1516	0	SER	A 208	10.449	4.413	55.379	1.00 40.02
-	1517	N	ASN A	A 209	10.039	2.817	56.924	1.00 46.75
	1518	CA	ASN A	A 209	11.446	2.513	57.161	1.00 45.16
	1519	CB	ASN I	A 209	11.987	1.709	55.972	1.00 44.54
20	1520	CG	ASN A	A 209	13.424	1.310	56.151	1.00 44.36
	1521	ODI	L ASN A	A 209	13.830	0.867	57.223	1.00 47.22
	1522	ND2	ASN A	A 209	14.208	1.459	55.101	1.00 45.74
	. 1523	C	ASN A	A 209	12.302	3.767	57.402	1.00 42.89
	1524	0	ASN A	A 209	13.460	3.825	57.003	1.00 41.55
25 _.	1525	N	PHE A	A 210	11.725	4.756	58.079	1.00 39.22
	1526	CA	PHE F	1 210	12.399	6.024	58.365	1.00 37.27
	152 7	СВ	PHE A	210	11.457	7.183	58.032	1.00 38.93
	1528	CG	PHE A		12.001	8.538	58.390	1.00 38.93
20	1529		PHE A		13.245	8.957	57.920	1.00 39.50
30	1530	_	PHE A		11.251	9.419	59.157	1.00 39.49
	1531		PHE A		13.724	10.234	58.211	1.00 36.40
	1532		PHE A		11.723	10.687	59.448	1.00 37.74
	1533	CZ	PHE A		12.957		58.973	1.00 37.09
25	1534	С	PHE A				59.815	1.00 35.77
33	1535	0		210	12.034		60.724	1.00 37.28
	1536	N	LEU A		14.165	6.135	60.024	1.00 30.72
	1537	CA	•	211	14.740		61.356	1.00 29.17
	1538	СВ		211	14.562	7,710	61.849	1.00 30.75
40	1539	CG	LEU A			8.795	61.043	1.00 31.54
40	1540		LEU A		14.887	10.158	61.551	1.00 30.37
	1541			211			61.149	1.00 29.89
	1542	С		211				1.00 28.83
	1543	0	LEU A	211	13.727	5.666	63.461	1.00 30.11

	1544	N	PRO, A	212	14.144	3.989	62.038	1.00 21.34
	1545	CD	PRO A	212	14.827	3.341	60.910	1.00 25.09
	1546	CA	PRO A	212	13.594	2.992	62.950	1.00 20.84
	1547	СВ	PRO A	212	13.783	1.686	62.182	1.00 24.56
5	1548	CG	PRO A	212	15.013	1.931	61.407	1.00 25.67
	1549	С	PRÒ A	212	14.275	2.986	64.311	1.00 19.94
	1550	0	PRO A	212	13.606	2.967	65.341	1.00 17.23
	1551	N	TRP A	213	15.607	3.016	64.308	1.00 28.93
•	1552	CA	TRP A	213	16.364	3.005	65.550	1.00 28.92
10	1553	СВ	TRP A	213	17.858	2.729	65.280	1.00 27.61
	1554	CG	TRP A	213	18.739	2.778	66.544	1.00 27.10
	1555	CD2	TRP A	213	19.294	1.661	67,264	1.00 27.80
	1556	CE2	TRP A	213	19.977	2.186	68.395	1.00 25.65
	1557	CE3	TRP A	213	19.277	0.271	67.071	1.00 27.47
15	1558	CD1	TRP A	213	19.106	3.896	67.253	1.00 25.51
	1559	NE1	TRP A	. 213	19.843	3.547	68.362	1.00 25.34
	1560	CZ2	TRP A	213	20.634	1.369	69.325	1.00 26.78
	1561	CZ3	TRP A	213	19.927	-0.537	67.997	1.00 27.71
	1562	CH2	TRP A	. 213	20.600	0.018	69.114	1.00 26.89
20	1563	С	TRP A	. 213	16.206	4.322	66.307	1.00 29.52
	1564	0	TRP A	213	15.844	4.325	67.479	1.00 30.08
	1565	N	GLN A	214	16.461	5.436	65.626	1.00 25.53
	1566	CA	GLN A	214	16.397	6.752	66.244	1.00 27.09
	1567	· CB	GLN A	214	16.892	7.820	65.265	1.00 32.69
25	1568	CG	GLN A	214	18.366	7.748	64.882	1.00 31.73
	1569	CD	GLN A	214	18.632	6.807	63.743	1.00 33.51
	1570	OE1	GLN A	214	19.768	6.664	63.304	1.00 31.73
	1571	NE2	GLN A	214	17.588	6.148	63.254	1.00 35.57
	1572	С	GLN A	214	15.039	7.176	66.763	1.00 29.77
30	1573	0	GLN A	214	14.952	7.775	67.830	1.00 30.98
	1574	N	GLY A	215	13.979	6.872	66.012	1.00 31.51
	1575	CA	GLY A	215	12.636	7.283	66.414	1.00 29.71
	1576	С	GLY A	215	11.951	6.363	67.397	1.00 30,52
	1577	0	GLY A	215	10.723	6.406	67.593	1.00 30.83
35	1578	N	ALA A	216	12.769	5.536	68.032	1.00 27.55
	1579	CA	ALA A	216	12.288	4.564	68.982	1.00 26.70
	1580	CB	ALA A	216	13.457	3.904	69.675	1.00 23.13
	1581	С	ALA A	216	11.335	5.186	69.980	1.00 27.72
	1582	0	ALA A	216	10.348	4.574	70.351	1.00 28.13
40	1583	N	TYR A	217	11.608	6.407	70.417	1.00 31.29
	1584	CA	TYR A	217	10.696	7.033	71.369	1.00 33.23
	1585	CB	TYR A	217	11.362	7.203	72.725	1.00 36.13
	1586	CG	TYR A	217	11.285	5.961	73.584	1.00 36.90

	1587	CD1	TYR	217		12.329	5.033	73.619	1.00	35.40
	1588	CE1	TYR F	217		12.241	3.899	74.421	1.00	39.13
	1589	CD2	TYR A	217	4	10.153	5.717	74.366	1.00	38.96
	1590	CE2	TYR	217		10.052	4.593	75.165	1.00	38.12
5	1591	CZ	TYR A	217		11.093	3.687	75 ⁻ .197	1.00	40.37
	1592	ОН	TYR A	217	•	10.976	2.595	76.032	1.00	39.19
	1593	С	TYR A	217	•	10.155	8.356	70.914	1.00	32.99
	1594	0	TYR A	217		9.539	9.073	71.687	1.00	34.63
	1595	N	SER A	218	1	10.375	8.659	69.643	1.00	29.75
10	1596	CA	SER A	218		9.933	9.904	69.054	1.00	32.78
	1597	СВ	SER A	218		10.368	9.977	67.592	1.00	51.24
	1598	OG	SER A	218		11.777	9.986	67.465	1.00	56.29
	1599	С	SER A	218	•	8.429	10.009	69.123	1.00	34.88
	1600	0	SER A	218		7.734	9.020	68.899	1.00	,35.86
15	1601	N	GLU A	219		7.927	11.199	69.453	1.00	50.24
	1602	CA	GLU A	219	,	6.487	11.431	69.495	1.00	51.43
	1603	·CB	GLU A	. 219		6.170	12.752	70.184	1.00	42.72
	1604	CG	GLU A	219		6.133	12.682	71.698	1.00	42.50
	1605	CD	GLU A	. 219		4.957	11.880	72.219	1.00	44.60
20	1606	OE1	GLU A	219		3.985	11.711	71.458	1.00	45.34
	1607	OE2	GLU A	219		4.992	11.430	73.386	1.00	45.20
	1608	С	GLU A	219		6.072	11.485	68.031	1.00	52.41
	1609	0	GLU A	219		6.756	12.076	67.206	1.00	52.72
	1610	N	LEU A	220		4.958	10.861	•	1.00	39.96
25	1611	CA		220	•	4.515	10.819	**	1.00	40.25
	1612	СВ	LEU A			4.058	9.395			26.28
	1613	CG	LEU A			5.132		66.411	1.00	19.24
	1614		LEU A			4.691		66.044		19.92
20	1615		LEU A			6.427		65.703		15.40
30	1616	С	LEU A			3.404	11.806	66.040		44.14
	1617	0	LEU A				12.072			
	1618	N	TYR A			3.402	12.358			53.92
	1619	CA	TYR A			2.366	13.304	64.443		57.45
25	1620	CB	TYR A			2.864	14.740			63.62
35	1621	CG	TYR A			1.885	15.812			66.26
	1622		TYR A			0.565	15.809	64.647		66.77
	1623		TYR A			-0.323	16.776	64.233		66.77
	1624		TYR A			2.282	16.824	63.339		67.06
40	1625		TYR A			1.400	17.788	62.926		67.52
40	1626	CZ	TYR A			0.106	17.758	63.373		67.28
	1627	OH	TYR A		-	-0.765	18.716	62.938		69.40
	1628	C	TYR A			1.924	13.074	•		58.86
	1629	0	TYR A	221		2.717	13.187	62.048	1.00	59.20

	1630	N	PHE		222	0.649	12.741	62.821	1.00	60.95
	1631	CA	PHE	A	222	0.089	12.490	61.503	1.00	62.79
	1632	СВ	PHE	A	222	-0.612	11.134	61.521	1.00	58.23
	1633	CG	PHE	. <u>.</u> .	222	0.307	9.989	61.848	1.00	58.94
5	1634	CD:	l PHE	À	222	0.060	9.167	62.945	1.00	58.55
	1635	CD2	2 PHE	A	222	1.438	9.743	61.071	1.00	58.48
	1636	CE	l PHE	A	222	0.923	8.123	63.265	1.00	58.44
	1637	CE2	2 PHE	A	222	2.303	8.704	61.384	1.00	56.86
	1638	CZ	PHE	A	222	2.043	7.893	62.486	1.00	58.47
10	1639	С	PHE	A	222	-0.879	13.600	61.066	1.00	64.53
•	1640	0	PHE	A	222	-1.436	14.312	61.897	1.00	65.86
	1641	N	THR	. A	223	-1.073	13.749	59.761	1.00	53.11
	1642	CA	THR	. A	223	-1.965	14.774	59.236	1.00	55.50
	1643	CB	THR	A	223	-1.342	16.165	59.311	1.00	74.89
15	1644	OG1	THR	A	223	-2.132	17.070	58.527	1.00	76.56
	1645	CG2	THR	A	223	0.091	16.146	58.765	1.00	75.02
	1646	С	THR	A	223	-2.299	14.542	57.778	1.00	56.91
	1647	0	THR	A	223	-1.409	14.522	56.926	1.00	57.65
	1648	N	ASP	A	224	-3.588	14.414	57.486	1.00	75.10
20	1649	CA	ASP	A	224	-4.050	14.176	56.124	1.00	75.82
	1650	СВ	ASP	A	224	-5.566	14.070	56.114	1.00	72.96
	1651	CG	ASP	A	224	-6.087	13.245	57.269	1.00	74.62
	1652	OD1	ASP	A	224	-6.195	13.791	58.389	1.00	76.73
	1653	OD2	ASP	A	224	-6.374	12.045	57.066	1.00	74.53
25	1654	С	ASP	A	224	-3.599	15.245	55.138	1.00	76.24
•	1655	0	ASP	A	224	-3.628	15.034	53.927	1.00	77.12
	1656	N	THR	A	225	-3.168	16.387	55.655	1.00	47.98
	1657	CA	THR	A	225	-2.719	17.478	54.807	1.00	49.10
•	1658	CB	THR	A	225	-2.165	18.619	55.655	1.00	84.57
30	1659	OG1	THR	A	225	-1.082	18.129	56.453	1.00	86.07
	1660	CG2	THR	A	225	-3.245	19.162	56.573	1.00	85.13
	1661	С	,		225	-1.636	17.020	53.849	1.00	48.17
	1662	0	THR			-0.790	16.225	54.216	1.00	49.64
	1663	N	LEU			-1.674	17.506	52.615	1.00	51.52
35	1664	CA	LEU			-0.657	17.143	51.636	1.00	52.64
	1665	CB	LEU			-1.046	17.626	50.237	1.00	72.33
	1666	CG	LEU			-1.979	16.711	49.441	1.00	72.59
	1667		LEU			-1.197	15.499		1.00	73.13
	1668		LEU.			-3.171	16.290	50.295	1.00	71.25
40	1669	С	LEU			0.616	17.825	52.097	1.00	53.19
	1670	0	LEU				18.561		1.00	53.08
	1671	N	TRP			1.725	17.610		1.00	66.66
	1672	CA	TRP	A	227	3.005	18.185	51.797	1.00	67.22

	1673	3 CE	3 TRP	A 2	27	4.16	9 17.28	9 51.35	3 1.00 60.56
	1674	C	TRP	A 2	27	5.518			
	1675	CE	2 TRP	A 2	27	5.99			
	1676	CE	2 TRP	A 2	27	7.29	1 18.995		
5	1677	CE	3 TRP	A 2	27	5.466	5 18.598		
	1678	CD	1 TRP	A 2	27	6.514			
	1679	NE	1 TRP	A 22	27	7.579	18.753		
	1680	CZ	2 TRP	A 22	:7	8.056	19.624	53.573	
	1681	CZ	3 TRP	A 22	:7	6.232	19.226	55.113	
10	1682	CH	2 TRP	A 22	7	7.511	. 19.729	54.826	•
	1683	С	TRP	A 22	7	3.311	19.618	51.392	1.00 68.58
	1684	0	TRP	A 22	7	3.833	20.385	52.195	1.00 68.87
	1685	N	PRO	A 22	8	3.034	19.999	50.142	1.00 87.77
4.7	1686	CD	PRO	A 22	8	2.724	19.233	48.927	1.00 98.49
15	1687	CA	PRO	A 22	8	3.349	21.391	49.810	1.00 88.87
	1688	CB	PRO			3.046	21.462	48.318	1.00 99.05
	1689	CG	PRO .			3.378		47.858	1.00 99.11
	1690	С	PRO .			2.468		50.637	1.00 88.93
20	1691	0	PRO I			2.716	23.530	50.717	1.00 88.53
20	1692	N	ASP A			1.448	21.736	51.260	1.00 95.84
	1693	CA	ASP A			0.490	22.450	52.105	1.00 95.31
	1694	CB	ASP A			-0.862	21.732	52.076	1.00 72.45
ı	. 1695	CG	ASP A			-1.597	21.940	50.779	
25	1696		ASP A			-2.571	21.198	50.517	1.00 73.15
, بد	1697		ASP A			-1.201	22.856	50.030	1.00 72.04
	1698 1699	С	ASP A			0.941	22.593	53.563	1.00 95.53
	1700	O N	ASP A			0.234	23.193		
	1701	CA	PHE A			2.103	22.033		
30	1702	CB	PHE A			2.616	22.122	55.246	1.00 69.91
	1703	CG	PHE A			3.607	20.983	-	1.00 60.91
	1704		PHE A			3.646	20.566		1.00 58.00
	1705		PHE A			2.548 4.756	19.941	57.566	1.00 55.95
	1706		PHE A			2.550	20.848	57.774	1.00 57.16
35	1707		PHE A			4.764	19.611 20.523	58.911	1.00 54.54
		CZ	PHE A			3.657	19.904	59.119	1.00 54.72
	1709	С	PHE A			3.303	23.473	59.687	1.00 54.36
		0	PHE A			4.409		55.349	1.00 69.25
			ASP A			2.616	24.407	54.837 56.008	1.00 67.25
40			ASP A			3.085	25.778	56.202	1.00105.50
			ASP A			· ' · · · · · · · · · · · · · · · · · ·	26.755	55.898	1.00105.80
			ASP A			0.672	26.438	56.683	1.00 68.25
			ASP A			-0.354		56.448	1.00 66.13
						- 1001	-,.100	50.448	1.00 66.14

	1716	00	2 ASP A 231	0.69	6 25.531	57.534	1.00 63.85
	1717	C	ASP A 231	3.59	26.022	57.617	1.00106.25
	1718	0	ASP A 231	3.44	1 25.169	58.493	1.00105.19
	1719	N	GLU A 232	4.19	8 27.185	57.837	1.00 75.85
5	1720	CA	GLU A 232	4.68	9 27.513	59,166	
	1721	CB	GLU A 232	5.08			
	1722	CG	GLU A 232	5.79	6 29.299		
	1723	CD	GLU A 232	6.24	9 30.743		
	1724	OE	1 GLU A 232	6.59	2 31.336	59.605	1.00 75.83
10	1725	OE	2 GLU A 232	6.28	4 31.276	61.788	
	1726	С	GLU A 232	3.53	5 27.246		
	1727	0	GLU A 232	3.71			
	1728	N	ALA A 233	2.33	8 27:617	•	
	1729	CA	ALA A 233	1.13	2 27.406	60.472	
15	1730	СВ	ALA A 233	-0.11	0 27.612	59.608	,
	1731	С	ALA A 233	1.16	4 25.980	60.987	
	1732	0	ALA A 233	1.14	5 25.733	62.195	1.00 66.72
	1733	N	ALA A 234	1.22	3 25.049	60.040	1.00105.33
	1734	CA	ALA A 234	1.26	3 23.627	60.332	1.00104.96
20	1735	CB	ALA A 234	1.37	2 22.840	59.036	1.00 70.15
	1736	С	ALA A 234	2.44	7 23.318	61.229	1.00104.98
	1737	0	ALA A 234	2.28	3 22.770	62.317	1.00105.25
	1738	N	LEU A 235	3.63	23.676	60.768	1.00 81.94
	1739	CA.	LEU A 235	4.843	3 23.427	61.536	1.00 81.18
25	1740	CB	LEU A 235	5.962	24.363	61.087	1.00 60.77
	1741	CG	LEU A 235	7.36	24.051	61.602	1.00 59.54
	1742		LEU A 235	7.388	24.143	63.099	1.00 59.47
	1743		LEU A 235	7.784	22.668	61.169	1.00 59.88
20	1744	С	LEU A 235	4.549	23.653	63.005	1.00 82.00
30	1745	0	LEU A 235	4.577	22.720	63.809	1.00 82.42
	1746	N	GLN A 236	4.258	24.901	63.351	1.00 79.63
	1747	CA	GLN A 236	3.968	25.252	64.735	1.00 79.41
	1748	CB	GLN A 236	3.717	26.758	64.864	1.00 86.03
25	1749	CG	GLN A 236	4.727		64.115	1.00 87.53
35	1750	CD	GLN A 236	4.724	29.069	64.564	1.00 88.57
	1751		GLN A 236	5.310		63.913	1.00 88.30
	1752		GLN A 236	4.075		65.688	1.00 90.39
	1753	С	GLN A 236		24.480	65.203	1.00 78.24
٠.	1754	0	GLN A 236		24.014	66.339	1.00 78.33
40	1755	N	GLU A 237	1.774		64.311	1.00 75.22
	1756	CA	GLU A 237		23.624	64.625	1.00 74.35
	1757	CB	GLU A 237		23.438	63.362	1.00 83.36
	1758	CG	GLU A 237	-1.792	23.489	63.582	1.00 85.49

	1759	e CI	GLU A	237	-2.290	22.464	64.592	2 1.00	86.68
	1760	O O	E1 GLU A	237	-1.986	22.616	65.796	5 1.00	87.49
	1761	L OI	E2 GLU A	237	-2.989	21.506	64.181	1.00	86.25
	1762	2 C	GLU A	237	0.945	22.269	65.199	1.00	73.31
5	1763	3 0	GLU A	237	0.373	21.810	66.189		72.96
	1764	N.	ALA A	238	1.937	21.636	64.580		68.54
	1765	CF	ALA A	238	2.418	20.337	65.043	1.00	67.12
	1766	CE	B ALA A	238	3.490	19.794	64.096	1.00	47.92
	1767	С	ALA A	238	3.001	20.507	66.440	1.00	65.44
10	1768	0	ALA A	238	2.659	19.769	67.368	1.00	64.92
	1769	N	ILE A	239	3.878	21.493	66.590	1.00	55.00
	1770	CA	ILE A	239	4.489	21.727	67.881	1.00	54.40
	1771	СВ	ILE A	239	5.429	22.917	67.829	1.00	40.35
	1772	CG	2 ILE A	239	6.326	22.929	69.059	1.00	39.90
15	1773	CG	1 ILE A	239	6.297	22.805	66.587	1.00	37.77
	1774	CD	1 ILE A	239	7.497	23.715	66.621	1.00	39.44
	1775	С	ILE A	239	3.426	21.939	68.955	1.00	56.09
	1776	0	ILE A	239	3.558	21.442	70.072	1.00	55.65
20	1777	· N	LEU A	240	2.363	22.663	68.624	1.00	65.76
20	1778	CA	LEU A		1.312	22.871	69.606	1.00	67.84
	1779	СВ	LEU A	240	0.124	23.614	68.990	1.00	93.15
	1780	CG	LEU A		-1.019	24.084	69.907	1.00	93.89
	. 1781		L LEU A		-2.066	24.781	69.047	1.00	94,06
٥.	1782	CD2	LEU A	240	-1.659	22.920	70.662	1.00	92.97
25	1783	С	LEU A 2		0.885	21.473	70.035	1.00	68.53
	1784	0	LEU A 2		0.593	21.226	71.205	1.00	68.37
	1785	N	ALA A 2		0.865	20.553	69.080	1.00	78.77
	1786	CA	ALA A 2		0.475	19.185	69.373	1.00	81.17
20	1787	CB	ALA A 2		0.189	18.439	68.082	1.00	73.59
30	1788	С	ALA A 2		1.561	18.464	70.171	1.00	82.11
	1789	0	ALA A 2		1.288	17.894	71.228	1.00	81.41
	1790	N	TYR A 2		2.789	18.496	69.665	1.00	68.88
	1791	CA	TYR A 2		3.914	17.838	70.329	1.00	69.93
25	1792	CB	TYR A 2		5.236	18.367	69.789	1.00	63.62
35	1793	CG	TYR A 2		6.402	18.047	70.678	1.00	61.34
	1794		TYR A 2		6.937	16.767	70.719	1.00	61.47
	1795		TYR A 2		8.002	16.465	71.565	1.00	60.57
	1796		TYR A 2		6.957	19.023	71.505	1.00	50.00
40	1797		TYR A 2		8.015	18.733	72.350	1.00 5	9.45
40	1798	CZ	TYR A 2		8.530	17.454	72.375	1.00 5	9.81
	1799	OH	TYR A 2		9.569	17.158	73.212	1.00 5	9.44
	1800	C	TYR A 2		3.893		71.831	1.00 7	2.10
	1801	0	TYR A 2	42	4.059	17.097	72.603	1.00 7	2.12

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	1846	CD	ARG A 247	3.868	8.005	80.558	1.00 96.03
	1847	NE	ARG A 247	3.758	6.592	80.920	1.00 96.92
	1848	CZ	ARG A 247	2.638	5.878	80.794	1.00 97.32
5	1849	· NH	11 ARG A 247	1.540	6.452	80.313	1.00 97.34
	1850	NH	2 ARG A 247	2.615	4.592	81.139	1.00 97.79
	1851	С	ARG A 247	7.688	9.168	78.571	1.00 79.63
	1852	0	ARG, A 247	7.713	8.084	79.165	1.00 78.61
	1853	N	ARG A 248	8.567	9.512	77.629	1.00154.67
10	1854	CA	ARG A 248	9.652	8.645		
	1855	СВ	ARG A 248	10.791	9.474	76.559	
	1856	CG	ARG A 248	10.540	9,967	75.143	1.00115.68
	1857	CD	ARG A 248	11.821	10.526	74.520	1.00116.07
	1858	NE	ARG A 248	11.612	11.027	73.160	1.00117.85
15	1859	CZ	ARG A 248	12.588	11.430	72.348	1.00118.27
	1860	NH:	1 ARG A 248	13.856	11.394	72.748	1.00118.12
	1861	NH	2 ARG A 248	12.294	11.873	71.134	1.00117.73
	1862	С	ARG A 248	10.256	7.722	78.204	1.00153.01
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40	1883	N	VAL A 252			85.529	1.00 71.62
40	1884	CA	VAL A 252	6.072	6.696	86.149	1.00 70.92
	1885	CB	VAL A 252	6.124		87.709	1.00 70.44
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	1887	CG2	VAL A 252	6.814	5.309	88.138	1.00 69.75

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	2039	CD	LYS		36		-10.473	8.005	84.014		100.22
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25	2041	NZ	LYS	В	36	•	9.350	10.106	83.267	1.00	98.40
	2042	С	LYS		36		-12.103	5.108	87.101	1.00	81.22
	2043	0	LYS	В	36		-13.009	5.559	87.795	1.00	80.91
	2044	N	ARG		37		-11.858	3.809	87.010	1.00	94.69
20	2045	CA	ARG	В	37		-12.666	2.848	87.741	1.00	95.89
30	2046	СВ	ARG	В	37		-12.681	1.518	86.984	1.00	94.83
	2047	CG	ARG		37		-13.043	1.673	85.510	1.00	93.94
	2048	CD	ARG		37		-13.101	0.340	84.768	1.00	93.08
	2049	NE	ARG		37		-14.256	-0.475	85.144	1.00	91.80
0.5	2050	CZ	ARG		37		-14.302	-1.294	86.190	1.00	90.45
35	2051		ARG		37		-13.250	-1.434	86.990	1.00	90.29
	2052	NH2	ARG		37		-15.415	-1.968	86.445	1.00	89.39
	2053	С	ARG		37			2.677	89.147	1.00	97.33
	2054	0	ARG		37		-12.011	1.569	89.687	1.00	97.61
40	2055	N	MET	В	38		-11.684	3.805	89.725	1.00	91.53
40	2056	CA	MET		38		-11.085	3.887	91.054	1.00	92.11
	2057	СВ	MET	В	38		-12.076	4.556	92.008	1.00	93.22
	2058	CG	MET	В	38		-12.462	5.948	91.530	1.00	94.17
	2059	SD	MET	В	38		-13.037	7.063	92.811	1.00	95.59

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	2354	CG	TRP		77	13.328	-3.151	85.188	1.00102.77
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	2358		TRP		7,7		-3.912	86.310	1.00103.91
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	2382	0	ARG	В	79	9.7	33 1.	026 89.	709 1.0	0 75.74
	2383	N	PRO	В	80	7.6	36 , 1.	800 90.	024 1.0	0 79.82
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	2402	CD	GLN		82	6.6				97.46
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2405 0	CINID	00	5 556 5 5		

	2404	NE	2 GLN	В 8	2	6.033	-5.106	97.575	1.00 97.19
	2405	C	GLN	B 8	2	5.756	-3.522	92.747	
,	2406	,0	GLN	в 8	2	- 5.577	-4.711	92.487	
	2407	N	GLŲ	В 8	3 [5.359	-2.551	91.932	1.00120.68
5	2408	CA	GLU	B) 8	3	4.778	-2.909	90.648	
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	2410	CG	GLU	B 8	3 ·	3.731	-1.984	88.508	1.00 93.63
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	2412	OE	1 GLU	B 8	3 .	3.083	-0.849	86.521	1.00 93.84
10	2413	OE:	2 GLU	B 83	3	3.267	0.346	88.340	1.00 94.14
	2414	С	GLÜ	B 83	3	5.996	-3.545	89.978	1.00120.39
	2415	0	GLU	B 83	3 .	7.087	-3.506	90.546	1.00121.16
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	2417	CA	VAL	B 84		6.951	-4.774	88.089	1.00100.63
15	2418	CB	VAL	B 84		8.197	-3.844	87.882	1.00 66.48
	2419		L VAL			7.812	-2.385	88.071	1.00 65.73
	2420	CG2	VAL	B 84		9.342	-4.253	88,806	1.00 65.12
	2421	С	VAL	B 84		7.366	-6.000	88.902	1.00100.20
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20	2423	N	LYS		,	7.323	-5.866	90.223	1.00100.82
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	2426	CG	LYS			7.988	-7.552	93.577	1.00 90.50
25	2427	CD	LYS		7.	8.244		94.942	1.00 92.14
23	2428 2429	CE	LYS			8.266	-7.970	96.056	1.00 92.89
	2429	NZ	LYS			8.412	-7.328	97.397	1.00 92.61
	2430	С	LYS I			6.335	-7.742	91.065	1.00 99.73
	2432	O	LYS I			6.316	-8.970	91.066	1.00 99.77
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	2435	CG	PHE E			2.893	-6.409	91.278	1.00113.66
	2436		PHE E			1.509 0.714	-6.649	90.743	1.00114.40
	2437		PHE E			1.001	-7.668	91.255	1.00114.81
35	2438		PHE E			-0.571	-5.851	89.724	1.00114.98
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	2592	СВ	ALA	В	104	-8.442	-25.377	75.402	1.00	71.86
	2593	С	ALA	В	104	-7.707	-25.041	73.039	1.00	62.67
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20	2595	N	ASN	В	105	-7.226	-23.861	72.656	1.00	47.98
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	2597	CB	ASN	В	105	-7.847	-21.811	71.446	1.00	54.12
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	2599	OD1	ASN	В	105	-9.745	-20.387	71.704	1.00	59.11
25	2600	ND2	ASN	В	105	-9.935	-22.483	72.472	1.00	55.23
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	2602	0	ASN	В	105	-6.677	-23.164	69.158	1.00	41.89
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	2614	CG1	VAL	В	107	-1.866	-19.142	71.395	1.00	40.11
40	2615	CG2	VAL	В	107	-4.224	-19.699	70.861	1.00	39.98
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	2965	CG	GL	JE	3 152		15.466	-7.801	68.769	1.00	24.82
	2966	CD	GL	jE	3 152		14.049	-8.044	68.279	1.00	26.88
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	3005		LEU				22.970	-5.888	63.735		50.05

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	3011	CG	LYS B 1	158	26.881	-9.954	70.828		56.65
	3012	CI	LYS B 1	158	27.413	-9.295	72.074		60.75
	3013	CE	LYS B 1	158	26.296	-8.885	73.014		62.28
	3014	NZ	LYS B 1	158	26.847	-8.245	74.244		65.28
10	3015	С	LYS B 1	158	26.568	-10.240	67.975		43.87
•	3016	0	LYS B 1	.58	27.272	-10.373	66.974		43.58
	3017	N	LEU B 1	.59	25.916	-11.248	68.552		53.59
	3018	CA	LEU B 1	.59	25.998	-12.620	68.058		53.87
	3019	CB	LEU B 1	.59	24.619	-13.263	68.079		38.71
15	3020	CG	LEU B 1	.59	24.051	-13.478	69.476		38.21
	3021	CD	1 LEU B 1	59	22.584	-13.874	69.409		38.39
	3022	CD	2 LEU B 1	59	24.852	-14.540	70.160		36.39
	3023	С	LEU B 1	59	26.569	-12.682	66.651		55.69
	3024	0	LEU B 1	59	27.526	-13.408	66.408		54.95
- 20	3025	N	ILE B 1	60	25.980	-11.928	65.723		47.80
	3026	CA	ILE B 1	60	26.484	-11.895	64.356		50.45
	3027	CB	ILE B 1	60	25.859	-10.715	63.523		52.45
	3028	CG	2 ILE B 1	60	26.733	-10.390	62.289		49.79
	3029	CG1	L ILE B 1	60	24.442	-11.074	63.070		52.17
25	3030	CD1	L ILE B 1	60	23.799	-10.012	62.178		50.29
	3031	С	ILE B 1	60	28.002	-11.709	64.426	1.00	52.81
	3032	0 .	ILE B 16	60	28.758	-12.637	64.144	1.00	53.75
	3033	N	SER B 16	61	28.434	-10.512	64.816	1.00	68.73
20	3034	CA	SER B 16	51	29.856	-10.180	64.923	1.00	70.90
30	3035	CB	SER B 16	_	30.044	-8.927	65.773	1.00	54.73
	3036	OG	SER B 16		29.664	-9.186	67.115	1.00	55.27
	3037	С	SER B 16		30.657	-11.325	65.535	1.00	72.09
	3038	0	SER B 16		31.708	-11.702	65.017	1.00	72.60
0.5	3039	N	GLN B 16		30.178	-11.862	66.652	1.00	65.45
35	3040	CA	GLN B 16		30.866	-12.987	67.270	1.00	67.74
	3041	СВ	GLN B 16		29.983	-13.639	68.343	1.00	74.56
	3042	CG	GLN B 16		30.507	-14.968	68.915	1.00	75.31
	3043	CD	GLN B 16		31.504	-14.788	70.050	1.00	76.13
40	3044		GLN B 16		31.219		71.042	1.00	76.95
40	3045		GLN B 16		32.672		69.911	1.00	75.35
	3046	С	GLN B 16		31.086		66.120	1.00 (59.54
	3047	0	GLN B 16		32.216 -	-14.218	65.703	1.00	70.50
	3048	N	ASP B 16	3	29.984 -	-14.483	65.589	1.00 7	78.04

	3049	CA	ASP	В	163	30.041	-15.425	64.485	1.00	79.04
	3050	СВ	ASP	В	163	28.632	2 -15.686	63.947	1.00	82.10
	3051	CG	ASP	В	163	27.787	7 -16.498	64.915	1.00	84.42
	3052	OD1	ASP	В	163	26.603	3 -16.761	64.611	1.00	85.70
5	3053	OD2	ASP	В	163	28.313	3 -16.879	65.985	1.00	84.15
	3054	С	ASP	В	163	30.974	-14.950	63.376	1.00	79.30
	3055	0	ASP	В	163	31.689	-15.757	62.791	1.00	80.39
	3056	N	VAL	В	164	30.986	-13.653	63.086	1.00	67.38
	3057	CA	VAL	·B	164	31.882	2 -13.150	62.046	1.00	68.00
- 10	3058	CB	VAL	В	164	31.707	-11.641	61.800	1.00	68.44
	3059	CG1	VAL	В	164	32.401	-11.250	60.509	1.00	68.71
	3060	CG2	VAL	В	164	30.240	-11.282	61.757	1.00	68.53
	3061	С	VAL	В	164	33.289	-13.374	62.581	1.00	68.33
	3062	0	VAL	В	164	34.187	-13.823	61.866	1.00	66.84
15	3063	N	TEU	В	165	33.449	-13.070	63.863	1.00	80.97
	3064	CA	LEU	В	165	34.718	-13.216	64.553	1.00	82.49
	3065	CB	LEU	В	165	34.545	-12.846	66.035	1.00	79.80
	3066	CG			165	35.745	-12.475	66.916		80.26
	3067		LEU			36.689	-13.655	67.072		80.94
20	3068		LEU				-11.288	66.302	1.00	80.62
	3069	С			165		-14.650			82.96
	3070	0			165		-14.880	64.056		83.85
•	3071	N .			166		-15.617			68.73
25	3072	CA				34.746		•		69.37
25.	3073	CB			166		-17.838			107.54
	3074	CG	ASP				-17.388	67.000		109.41
	3075		ASP				-17.953	67.898		110.51
	3076		ASP			34.894		·		109.83
30	3077	C	ASP			34.649				68.95
50	3078	0	ASP				-18.798	63.055		68.96
	3079	N			167		-16.770			74.82
	3080 3081	CA	ALA				-17.202			73.74
		CB	ALA				-17.850	60.416		71.38
35	3082 3083	С	ALA				-18.160			73.42
33	3084	O N	ALA LYS				-18.861			73.13
	3085	N CA	LYS				-18.193 -19.059	61.395		76.94
	3086	CB	LYS					61.209	•	76.07
	3087						-19.182	62.504		83.53
40	3088	CG CD	LYS				-19.542 -20.145			84.67
	3089	CE	LYS				-20.145	64.821		86.13
•	3099	NZ	LYS				-20.088 -18.706	66.201		85.76
							-18.706			86.00
	3091	С	LYS	D	T 00	30.638	-18.476	60.109	1.00	75.99

	3092	0.	LYS B 168	29.787 -19.	168 59.556	1.00	76.10
	3093	N	ILE B 169	30.831 -17.	195 59.809	1.00	56.33
	3094	CA	ILE B 169	30.091 -16.	516 58.743	1.00	56.70
	3095	СВ	ILE B 169	28.740 -15.	943 59.224	1.00	88.89
5	3096	CG	2 ILE B 169	27.906 -17.	042 59.851	1.00	89.46
	3097	CG	1 ILE B 169	28.969 -14.	811 60.224	1.00	88.80
	3098	CD	1 ILE B 169	27.695 -14.	129 60.677	1.00	89.12
	3099	С	ILE B 169	30.969 -15.	375 58.243	1.00	56.55
	3100	0	ILE B 169	32.035 -15.	131 58.799	1.00	56.78
10	3101	N	ASN B 170	30.527 -14.	663 57.213	1.00	71.19
	3102	CA	ASN B 170	31.347 -13.	584 56.672	1.00	71.78
	3103	CB	ASN B 170	31.795 -13.	965 55.259	1.00	79.14
*	3104	CG	ASN B 170	33.252 -13.	655 55.001	1.00	78.99
	3105	OD:	1 ASN B 170	34.140 -14.	169 55.688	1.00	79.74
15	3106	ND	2 ASN B 170	33.509 -12.	818 54.000	1.00	78.04
	3107	С	ASN B 170	30.690 -12.	200 56.646	1.00	71.52
	3108	0	ASN B 170	29.479 -12.	072 56.457	1.00	70.38
	3109	N	PRO B 171	31.496 -11.	140 56.820	1.00	79.18
	3110	CD	PRO B 171	32.952 -11.	187 57.033	1.00	96.01
20	3111	CA	PRO B 171	31.020 -9.	753 56.819	1.00	78.61
	3112	CB	PRO B 171	32.280 -8.9	956 57.147	1.00	96.07
	3113	CG	PRO B 171	33.373 -9.8	314 56.592	1.00	97.33
	3114	С	PRO B 171	30.374 -9.3	330 55.500	1.00	77.50
	3115	0	PRO B 171	29.636 -8.3	348 55.447	1.00	78.36
25	3116	N	GLY B 172	30.660 -10.0	064 54.434 ·	1.00	73.27
	3117	CA	GLY B 172	30.049 -9.7	747 53.158	1.00	70.47
	3118	С	GLY B 172	28.684 -10.4	118 53.117	1.00	68.95
	3119	0	and the second s	27.865 -10.1		1.00	68.33
•	3120	N		28.448 -11.2			61.89
30	3121	CA		27.192 -12.0	009 54.218	1.00	58.97
	3122	CB	ASP B 173	27.444 -13.4		1.00	67.48
	3123	CG		28.349 -14.2			68.30
	3124		ASP B 173	27.992 -14.4	13 52.658	1.00	68.23
0.5	3125			29.415 -14.6		1.00	67.70
35	3126	С	ASP B 173	26.261 -11.2		1.00	56.51
	3127	0		25.234 -11.8			56.63
	3128	N	ILE B 174	26.636 -10.0		1.00	58.22
	3129	CA		25.822 -9.2	93 56.463	1.00	55.66
40	3130	CB	ILE B 174	26.659 -8.2		1.00	48.35
40	3131		ILE B 174	25.753 -7.3		1.00	47.15
	3132		ILE B 174	27.658 -8.9		1.00	45.67
	3133			28.680 -7.9		1.00	45.81
	3134	С	ILE B 174	24.758 -8.5	71 55.665	1.00	53.97

	3135	0	ILE	В 174	25.039	-7.617	54.942	1.00 53.77
	3136	N	THR	в 175	23.524	-9.023	55.804	1.00 50.65
•	3137	CA	THR	в 175	22.438	-8.404	55.078	1.00 48.25
	3138	СВ	THR :	B 175	22.167	-9.189	53.814	1.00 47.89
5	3139	OG	1 THR	в 175	22.080	-10.579	54.141	1.00 47.65
	3140	CG.	2 THR	в 175	23.292	-8.990	52.830	1.00 47.35
	3141	С	THR I	В 175	21.157	-8.277	55.894	1.00 47.27
	3142	0	THR	3 175	20.968	-8.952	56.907	1.00 48.30
	3143	N	GLU I	3 176	20.283	-7.387	55.449	1.00 40.67
10	3144	CA	GLU I	3 176	19.031	-7.171	56.133	1.00 38.01
	3145	CB	GLU I	3 176	18.082	-6.378	55.237	1.00 38.17
	3146			3 176	18.450	-4.914	55.152	1.00 39.37
	3147			3 176	17.625	-4.123	54.157	1.00 41.38
	3148		L GLU E		16.373	-4.180	54.216	1.00 42.98
15	3149	OE2	2 GLU E		18.247	-3.431	53.319	1.00 42.31
	3150	С	GLU E		18.425	-8.505	56.514	1.00 38.12
	3151	0	GLU E			-8.724		1.00 37.44
	3152	N	GLU E			-9.409	55.548	1.00 43.72
20	3153	CA	GLU E			-10.713	55.812	1.00 46.24
20	3154		GLU E			-11.595		1.00 86.81
	3155	CG	GLU E			-13.019		1.00 95.81
	3156	CD	GLU B			-13.921		1.00100.82
	3157		GLU B			-14.011		1.00103.81
25	3158		GLU B			-14.548	•	1.00101.00
25	3159	C	GLU B			-11.380		1.00 44.23
	3160	0	GLU B			-11.859		1.00 44.32
	3161	N	LEU B			-11.410		1.00 41.63
	3162	CA	LEU B					1.00 38.74
30	3163 3164	CB CG	LEU B					1.00 44.89
50	3165		LEU B		23.040		58.803	1.00 44.18
	3166		LEU B		22.852			
	3167	C	LEU B			-11.493		1.00 43.37
	3168	0	LEU B		•	-11.493		1.00 36.74
35		N	ILE B			-12.244		1.00 35.45
	3170	CA	ILE B			-9.529		1.00 30.73
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	3172		ILE B		19.054			
	3173		ILE B				60.512	1.00 32.26
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	3175	C	ILE B			-10.021		1.00 28.71
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	3177	N	GLY B			-10.250		1.00 29.07
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	3266	CE	LYS	В	190	14.436	-16.857	56.654	1.00	67.52
,	3267	NZ	LYS	В	190	15.093	-17.892	55.793	1.00	67.17
5	3268	C .	LYS	В	190	8.902	-15.242	57.073	.1.00	45.92
	3269	0	LYS	В	190	9.076	-14.053	57.308	1.00	45.33
	3270	N ·	ASP	В	191	7.821	-15.682	56.453	1.00	41.73
	3271	CA	ASP	В	191	6.824	-14.733	55.996	1.00	41.48
	3272	СВ	ASP	В	191	5.856	-15.402	55.030	1.00	63.45
10	3273	CG	ASP	В	191	6.313	-15.294	53.592	1.00	67.43
	3274	OD1	ASP	В	191	5.676	-15.921	52.717	1.00	70.88
	3275	OD2	ASP	В	191	7.306	-14.577	53.329	1.00	69.09
	3276	С	ASP	В	191	6.042	-14.028	57.070	1.00	40.03
	3277	0	ASP	В	191	5.336	-13.078	56.775	1.00	39.83
15	3278	N	LEU	В	192	6.168	-14.449	58.321	1.00	47.34
	3279	CA	LEU	В	192	5.387	-13.798	59.350	1.00	45.66
	3280	СВ	LEU	В	192	4.504	-14.831	60.040	1.00	38.64
	3281	CG	LEU	В	192	3.454	-15.563	59.196	1.00	36.65
	3282	CD1	LEU	В	192	2.572	-16.388	60.112	1.00	38.15
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	3284	С	LEU	В	192	6.144	-13.000	60.395	1.00	45.53
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	3291	NE	ARG	В	193	12.214	-14.948	60.547	1.00	44.54
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	3296	0	ARG	В	193	7.876	-10.083	62.494	1.00	35.46
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35	3298	CA	ASP	В	194	7.169	-8.487	60.382	1.00	43.32
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	3300	CG	ASP	В	194	9.076	-7.825	58.881	1.00	40.95
	3301	OD1	ASP	В	194	9.820	-8.219	59.810	1.00	40.39
	3302	OD2	ASP	В	194	9.492	-7.500	57.751	1.00	42.29
40	3303	С	ASP	В	194	5.678	-8.308	60.532	1.00	42.96
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	3305	N	PRO	В	195	5.248	-7.415	61.429	1.00	34.18
	3306	CD	PRO	В	195	5.994	-6.877	62.572	1.00	31.05

	3307	CA	PRO	В	195	3.824	-7.177	61.626	1.00	33.33
	3308	СВ	PRO	В	195	3.795	-6.376	62.923	1.00	28.62
	3309	CG	PRO	В	195	4.930	-6.870	63.642	1.00	30.37
	3310	С	PRO	В	195	3.271	-6.362	60.469	1.00	32.39
5	3311	0	PRO	В	195	3.950	-5.469	59.973	1.00	33.28
	3312	N.	ASP	В	196	2.040	-6.658	60.049	1.00	33.82
	3313	CA	ASP	В	196	1.407	-5.894	58.967	1.00	33.08
	3314	СВ	ASP	В	196	0.356	-6.723	58.213	1.00	40.99
	3315	CG	ASP	В	196	0.898	-8.031	57.676	1.00	41.96
10	3316	OD1	ASP	В	196	1.002	-9.013	58.450	1.00	42.06
	3317	OD2	ASP	В	196	1.215	-8.063	56.467	1.00	43.06
	3318	С	ASP	В	196	0.685	-4.704	59.599	1.00	31.99
	3319	0	ASP	В	196	0.508	-3.652	58.973	1.00	31.68
	3320	N	LEU	В	197	0.281	-4.888	60.851	1.00	40.44
15	3321	CA	LEU	В	197	-0.448	-3.867	61.578	1.00	41.69
	3322	CB	LEU	В	197	-1.941	-4.217	61.522	1.00	39.81
	3323	CG	LEU	В	197	-2.962	-3.590	62.471	1.00	38.39
	3324	CD1	LEU	В	197	-3.375	-2.208	61.983	1.00	34.37
	3325	CD2	LEU	В	197	-4.163	-4.514	62.546	1.00	40.85
20	3326	С	LEU	В	197	0.019	-3.762	63.031	1.00	42.42
	3327	0	LEU	В	197	-0.003	-4.757	63.764	1.00	42.95
	3328	N	ILE	В	198	0.445	-2.564	63.438	1.00	34.38
	3329	CA	ILE	В	198	0.887	-2.335	64.807	1.00	35,.37
	3330	CB	ILE	В	198	2.266	-1.644	64.850	1.00	26.32
25 ·	3331	CG2	ILE	В	198	2.471	-0.929	66.202	1.00	23.20
	3332	CG1	ILE	В	198	3.359	-2.690	64.602	1.00	23.88
	3333	CD1	ILE	В	198	4.757	-2.179	64.832	1.00	18.24
	3334	С	ILE			-0.141	-1.456	65.484	1.00	36.77
	3335	0	ILE			-0.430	-0.369	64.981		37.04
30	3336	N	ILE	В	199	-0.668	-1.926	66.621	1.00	41.16
	3337	CA	ILE			-1.721	-1.240	67.400		43.74
	3338	CB	ILE			-2.941	-2.196	67.652		49.23
	3339		ILE			-3.835	-1.671	68.767		45.95
25	3340		ILE			-3.760	-2.355	66.383		47.61
35	3341		ILE			-4.875	-3.363	66.540		49.10
	3342	С	ILE			-1.315	-0.703	68.771		44.54
	3343	0	ILE			-0.899	-1.468	69.652		45.29
	3344	N	ARG			-1.479	0.608	68.953		36.74
40	3345	CA	ARG			-1.182	1.270	70.230		37.18
40	3346	CB	ARG			-0.257		70.041		44.70
	3347	CG	ARG			0.216	3.120	71.367		45.83
	3348	CD	ARG			0.776		72.313		46.69
	3349	NE	ARG	В	200	1.375	2.561	73.549	1.00	50.52

	2250	08	7 D.C	р	200		2.447	3 348	73.608	1.00	49.70
	3350	CZ	ARG				3.055		72.496		50.01
	3351		ARG ARG				2.923		74.787		49.31
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5	3353	C					-3,154	1.00	70.142		34.80
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*	3357	СВ	THR				-4.562	٠,	74.583		26.30
10	3358	OG1					-3.507	0.517	72.999		24.68
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15	3364	CB			202	•	-4.196		76.561		68.80
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22	3373	CA			204		-0.674		72.510		41.03
25	3374	CB			204		-0.020		73.446		42.47
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	3382	CA			205			8.543	69.424		39.70
~-	3383	CB			205		1.054		68.586		35.62
35	3384	CG			205		-0.410		68.185		35.68
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	3386		LEU				-1.150	8.712			33.17
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	3388	0			205		3.674		69.068		39.65
40	3389	N			206		3.233	7.138	70.005		38.80
	3390	CA			206		4.626		70.115		40.82
	3391	CB			206		5.175		71.464		46.44
	3392	CG	ARG	В	206		4.403	6.733	72.680	1.00	49.25

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	3400	N	LEU	E	207		5.901	4.714	69.694	1.00	40.36
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	3404	CD1	LEU	В	207		6.712	3,206	65.771	1.00	37.88
	3405	CD2	LEU	В	207		5.166	1.634	66.949	1.00	37.85
	3406	С	LEU	В	207		6.835	2.684	70.700	1.00	37.93
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	3409	CA	SER	В	208		7.930	3.140	72.821	1.00	40.20
	3410	СВ	SER	В	208		6.946	2.888	73.963	1.00	42.07
	3411	OG	SER	В	208		6.207	4.066	74.244	1.00	43.06
20	3412	С	SER	В	208		8.858	1.933	72.634	1.00	39.55
•	3413	0	SER	В	208		8.811	0.973	73.396	1.00	37.18
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	3415	CA	ASN	В	209	<i>:</i>	10.670	0.968	.,71.306	1.00	30.52
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	3418	OD1	ASN	В	209		13.800	-0.097	72.808	1.00	27.06
	3419	ND2	ASN	В	209		13.372	0.730	70.790	1.00	26.24
	3420	С	ASN	В	209		10.088	-0.410	71.006	1.00	29.69
	3421	0	ASN	В	209		10.634	-1.424	71.434	1.00	30.39
30	3422	N	PHE	В	210		8.997	-0.463	70.258	1.00	31.34
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	3424	СВ	PHE	В	210		6.864	-1.663	70.147	1.00	33.86
	3425	CG	PHE	В	210		6.155	-2.984	70.058	1.00	35.91
	3426	CD1	PHE	В	210		6.340	-3.956	71.032	1.00	33.45
35	3427	CD2	PHE	В	210		5.266	-3.242	69.020	1.00	36.79
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	3429	CE2	PHE	В	210		4.575	-4.444	68.964	1.00	33.34
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	3479	0	ALA	В 21	6		8.853	0.871	58.332	2 1.0	0 29.21
	3480) N	TYR	B 21	7,	•	7.827	-1.135	58.362	1.0	0 33.05
	3481	CA	TYR	B 21	7		6.859	-0.762	57.337	1.0	0 33.52
	3482	CB	TYR'	B 21	7		7.129	-1.456	56.006	1.0	0 26.97
5	3483	CG	TYR	B 21	7		8.494	-1.239	55.375	1.0	0 27.03
	3484	CD:	1 TYR	B 21	7		9.606	-2.025	55.751		0 28.49
	3485	CE:	1 TYR	B 217	7		10.823	-1.913	55.083	1.0	26.38
	3486	CD2	2 TYR	B 217	,		8.657	-0.332	54.325	1.00	27.94
	3487	CE	2 TYR	B 217	, '		9.867	-0.217	53.658	1,.00	29.81
10	3488	CZ	TYR	B 217			10.936	-1.012	54.036	1.00	30.32
	3489	ОН	TYR	B 217			12.096	-0.935	53.320	1.00	35.46
	3490	С	TYR	B 217			5.435	-1.091	57.710	1.00	35.00
	3491	0	TYR	B 217			4.535	-0.940	56.881	1.00	37.26
	3492	N	SER	B 218			5.202	-1.544	58.935	1.00	31.38
15	3493	CA		B 218			3.835	-1.880	59.312	. 1.00	34.90
	3494	CB		B 218		•	3.823	-2.590	60.667	1.00	44.37
	3495	OG	SER :	B 218			4.843	-2.094	61.506	1.00	49.79
	3496	С		B 218			2.885	-0.686	59.316	1:00	34.66
20	3497	0		B 218				0.460	59.255	1.00	35.96
20	3498	N		B 219	,		1.586	-0.980	59.345	1.00	46.39
	3499	CA		B 219				0.042	59.376	1.00	48.11
	3500	CB		3 219			-0.780	-0.477	58.787	1.00	42.82
	3501	CG		3 219	2.	٠, ٠	-0.765	-0.799	57. 295	1.00	40.25
25	3502	CD	GLU I				-0.760				41.75
25	3503		GLU E				0.641		56.965		41.05
•	3504	OE2					0.869		55.185		43.48
	3505	C	GLU E				0.305				48.55
	3506	0	GLU E				0.145	-0.566	61.651		49.82
30	3507	N	LEU E				0.279	1.623	61.168		42.65
50	3508	CA	LEU E					1.981			
	3509 3510		LEU B				0.892				
	3511	CG CD1	LEU B				2.283				31.02
	3512		LEU B				2.922				29.61
35	3513		LEU B						63.320		32.36
	3514		LEU B						62.769		46.39
	3515		TYR B				2.089 1.882	2.722	61.867		47.21
	3516		TYR B				3.278	1.929	63.964		53.95
	3517		TYR B						64.310		55.64
40	3518		TYR B				5.529	0.923 1.036	63.976		58.57
- •	3519		TYR B				5.329		64.477		60.14
									64.026		59.26
			TYR B				6.012		64.518 65.430	1.00	
		-				(0.100	05.430	1.00	ρ1.11

	3522	CE2	TYR	В	221	-7.294	0.274	65.930	1.00	62.90
	3523	CZ	TYR	В	221	-8.116	1.283	65.476	1.00	62.23
	3524	OH	TYR	В	221	-9.384	1.397	66.009	1.00	60.46
	3525	С	TYR	В	221	-3.451	2.471	65.781	1.00	57.07
5	3526	0	TYR	В	221	-3.361	1.586	66.639	1.00	58.08
	3527	N	PHE	В	222	-3.710	3.749	66.050	1.00	56.47
	3528	CA	PHE	В	222	-3.912	4.262	67.402	1.00	57.27
	3529	СВ	PHE	В	222	-3.249	5.630	67.548	1.00	49.96
	3530	CG	PHE	В	222	-1.891	5.695	66.946	1.00	48.78
10	3531	CD1	PHE	В	222	-1.735	5.891	65.589	1.00	47.54
	3532	CD2	PHE	В	222	-0.760	5.524	67.731	1.00	49.19
	3533	CE1	PHE	В	222	-0.476	5.916	65.019	1.00	48.43
	3534	CE2	PHE	В	222	0.504	5.547	67.167	1.00	46.75
	3535	CZ	PHE	В	222	0.643	5.744	65.810	1.00	47.56
15	3536	С	PHE	В	222	-5.393	4.387	67.762	1.00	58.98
	3537	0	PHE	В	222	-6.233	4.773	66.937	1.00	59.22
	3538	N	THR	В	223	-5.700	4.074	69.013	1.00	65.91
	3539	CA	THR	В	223	-7.064	4.137	69.491	1.00	66.56
	3540	CB	THR	В	223	-7.710	2.747	69.429	1.00	68.79
20	3541	OG1	THR	В	223	-9.101	2.874	69.729	1.00	73.73
	3542	CG2	THR	В	223	7.054	1.784	70.423	1.00	66.05
	3543	С	THR	В	223	-7.092	4.667	70.921	1.00	67.20
	3544	0	THR	В	223	-6.491	4.077	71.823	1.00	68.64
	3545	N	ASP	В	224	-7.793	5.780	71.126	1.00	59.07
25	3546	CA	ASP	В	224	-7.875	6.392	72.450	.1.00	57.77
•	3547	CB	ASP	В	224	-8.771	7.641	72.413	1.00	59.96
	3548	CG	ASP		,	-8.166	8.766	71.589	1.00	62.19
	3549		ASP			-7.818	8.503	70.421	1.00	64.70
••	3550		ASP	В	224	-8.031	9.903	72.095	1.00	61.88
30	3551	С	ASP			-8.340	5.461	73.569		56.76
	3552	0			224	-8.283		74.737	1.00	56.94
	3553	N			225	-8.781		73.235	1.00	40.23
	3554	CA			225	-9.243		74.275		41.21
0.5	3555	CB			225			73.710	1.00	69.35
35	3556				225	•		73.891		71.55
	3557				225			72.240	1.00	70.88
	3558	С	THR			-8.111	2.642	75.033		39.57
	3559	0			225	-7.111		74.443	1.00	38.26
40	3560		LEU			-8.288		76.343		49.79
40	3561	CA			226	-7.297		77.202		50.45
	3562		LEU			-7.552		78.679	1.00	
	3563	CG			226			79.135	1.00	¥
	3564	CD1	LEU	В	226	-6.975	3.744	80.476	1.00	73.87

		_									
	3565		LEU					4.5			73.91
	3566	С			226		-7.346				50.06
	3567	0	LEU	В	226		-8.382	-0.2			50.52
_	3568	N	TRP	В	227		-6.220	-0.3			56.52
5	3569	CA	TRP	В	227	,	-6.109	-1.7	49 77.03	31 1.00	55.63
	3570	CB	TRP	В	227		-4.836	-2.2	82 77.67	2 1.00	40.08
	3571	CG	TRP	В	227		-4.591	-3.7	10 77.34	3 1.00	32.65
	3572	CD2	TRP	В	227		-4.712	-4.3	36 .76.05	6 1.00	29.73
	3573	CE2	TRP	В	227		-4.357	-5.6	98 76.22	0 1.00	29.35
10	3574	CE3	TRP	В	227		-5.086	-3.88	32 74.77	8 1.00	30.04
	3575	CD1	TRP	В	227		-4.183	-4.68	32 78.20	2 1.00	32.68
	3576	NE1	TRP	В	227		-4.039	-5.87	77 77.54	1 1.00	31.63
	3577	CZ2	TRP	В	227	•	-4.362	-6.6	16 75.15	8 1.00	27.35
	3578	CZ3	TRP	В	227		-5.092	-4.80	02 73.71	4 1.00	27.85
15	3579	CH2	TRP	В	227		-4.729	-6.15	54 73.92	3 1.00	28.92
	3580	С	TRP	В	227		-7.272	-2.63	37 77.44	6 1.00	57.42
	3581	0	TRP	В	227		-7.930	-3.22	20 76.59	3 1.00	57.78
	3582	N	PRO	В	228		-7.550	-2.75	8 78.75	1 1.00	59.57
	3583	CD	PRO	В	228	-	-6.949	-2.13	38 79.94	2 1.00	82.42
20	3584	CA	PRO	В	228	-	-8.669	-3.63	34 79.13	1 1.00	61.06
	3585	CB	PRO	В	228	-	-8.747	-3.45	80.64	9 1.00	84.47
	3586	CG	PRO	В	228	-	-7.327	-3.12	9 81.02	2 1.00	83.95
i	3587	С	PRO	В	228		-9.997	,- 3.33	39 78.41	7 1.00	60.86
	3588	0	PRO	В	228	-1	10.852	-4.21	.0 78.27	8 1.00	59.30
25	3589	N	ASP	В	229	-1	10.157	-2.10	6 77.96	0 1.00	63.90
	3590	CA	ASP	В	229	-1	1.363	-1.71	77.25	7 1.00	65.67
	3591	СВ	ASP	В	229	-1	1.548	-0.20	3 77.32	4 1.00	66.08
	3592	CG	ASP	В	229	-1	1.601	0.31	0 78.74	1.00	67.12
	3593	OD1	ASP	В	229	-1	1.670	1.54	5 78.92	5 1.00	66.03
30	3594	OD2	ASP	В	229	-1	1.574	-0.52	7 79.66	9 1.00	66.23
	3595	С	ASP	В	229	-1	1.248	-2.14	7 75.80	5 1.00	66.75
	3596	0	ASP	В	229	-1	2.000	-1.68	1 74.95	0 1.00	67.93
	3597	N	PHE	В	230	-1	0.289	-3.02	1 75.52	3 1.00	69.70
	3598	CA	PHE	В	230	-1	0.096	-3.50	6 74.16	4 1.00	67.90
35	3599	СВ	PHE	В	230	_	8.606	-3.65	6 73.84	1.00	35.34
	3600	CG	PHE	В	230	_	8.283	-3.50	9 72.38	2 1.00	26.39
	3601	CD1	PHE	В	230	_	8.216	-2.26	2 71.80		21.82
	3602	CD2	PHE	В	230		8.033	-4.62	2 71.589		22.39
	3603	CE1	PHE	В	230		7.901	-2.11			18.61
40	3604		PHE					-4.47			17.21
	3605	CZ	PHE				7.654	-3.21			16.11
	3606	С	PHE					-4.85			70.82
	3607	0	PHE					-5.68			70.34
			_			_					

	3608	3 N	ASP B 23	1	-11.588	8 -5.065	73.085	1.00105.90
	3609	O CA	A ASP B 23	1	-12.36	5 -6.285	72.900	1.00107.50
	3610		3 ASP B 23	1	-13.78	1 -6.063	73.415	1.00 85.49
	3613	r co	ASP B 23	1	-14.412	2 -4.824	72.820	1.00 87.23
5	3612) OE	01 ASP B 23	1	-14.335	5 -4.670	71.582	1.00 86.76
	3613	O C	02 ASP B 23	1.	-14.973	3 -4.006	73.580	1.00 88.98
	3614	C	ASP B 23	1	-12.439	-6.660	71.426	1.00108.26
	3615	0	ASP B 23	1	-11.697	-6.135	70.601	1.00108.49
*	3616	N	GLU B 23	2	-13.372	2 -7.547	71.104	•
10	3617	CA	GLU B 23	2	-13.553	-8.016	69.740	
	3618	CB	GLU B 23	5.	-14.574	-9.143		
	3619	CG	GLU B 23	2	-14.395	-10.072	68.551	1.00 64.71
	3620	CD	GLU B 232	?	-15.119	-11.386	68.743	
	3621	OE	1 GLU B 232	?	-14.865	-12.066	69.766	
15	3622	OE:	2 GLU B 232	: .	-15.940	-11.737	67.868	
	3623	С	GLU B 232		-13.972	-6.925	68.761	1.00 61.20
	3624	0	GLU B 232		-13.516	-6.894	67.620	1.00 61.27
	3625	Ŋ	ALA B 233	•	-14.844	-6.027	69.197	1.00 70.90
	3626	CA	ALA B 233		-15.288	-4.949	68.318	1.00 73.06
20	3627	CB	ALA B 233		-16.464	-4.209	68.938	1.00 93.53
	3628	С	ALA B 233		-14.142	-3.979	68.065	1.00 73.31
	3629	0	ALA B 233		-14.200	-3.153	67.151	1.00 73.80
	3630	N	ALA B 234		-13.102	-4.086	68.888	1.00 71.16
~ ~	3631	CA	ALA B 234	6 A	-11.932	-3.217	68.777	1.00 70.00
25	3632	CB	ALA B 234		-11.236	-3.120	70.132	1.00 96.43
.,	3633	С	ALA B 234		-10.957	-3.741	67.725	1.00 67.92
	3634	0	ALA B 234		-10.543	-3.005	66.816	1.00 65.56
	3635	N	LEU B 235		-10.594	-5.015	67.871	1.00 55.18
20	3636	CA	LEU B 235		-9.678	-5.668	66.954	1.00 54.73
30	3637	CB	LEU B 235		-9.623	-7.170	67.238	1.00 48.95
	3638	CG	LEU B 235		-8.233	-7.803	67.303	1.00 48.32
	3639		LEU B 235		-8.335	-9.313	67.500	1.00 46.48
	3640		LEU B 235		-7.496	-7.479	66.035	1.00 47.32
25	3641	С	LEU B 235		-10.235	-5.431	65.567	1.00 56.02
35	3642	0	LEU B 235		-9.517	-5.035	64.643	1.00 54.95
	3643	N	GLN B 236		-11.543	-5.645	65.447	1.00 70.62
	3644	CA	GLN B 236		-12.244	-5.487	64.185	1.00 70.74
	3645	CB	GLN B 236		-13.666	-6.046	64.321	1.00 88.42
40	3646	CG	GLN B 236		-13.679	-7.553	64.590	1.00 92.34
40	3647	CD	GLN B 236		-15.072	-8.173	64.557	1.00 94.69
	3648		GLN B 236		-15.818	-8.002	63.591	1.00 95.25
	3649		GLN B 236			-8.912	65.611	1.00 94.26
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	3653	CA	GLU	В	237	-12.645	-1.703	63.957	1.00 52.29
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5	3655	CG	GLU	В	237	-13.056	0.756	64.605	1.00 78.85
	3656	CD	GLU	В	237	-14.097	1.005	63.514	1.00 81.46
	3657	OE1	GLU	В	237	-15.314	1.018	63.822	1.00 81.02
	3658	OE2	GLU	В	237	-13.690	1.184	62.342	1.00 81.65
	3659	С	GLU	В	237	-11.266	-1.397	63.413	1.00 51.87
10	3660	0	GLU	ъ	237	-11.099	-0.530	62.552	1.00 51,44
	3661	N	ALA	В	238	-10.287	-2.137	63.929	1.00 63.75
	3662	CA	ALA	В	238	-8.892	-1.999	63.532	1.00 62.12
	3663	СВ	ALA	В	238	-7.991	-2.450	64.657	1.00 66.94
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15	3665	0	ALA	·B	238	-8.329	-2.299	61.230	1.00 60.24
	3666	N	ILE	В	239	-8.758	-4.166	62.453	1.00 40.23
	3667	CA	ILE	В	239	-8.555	-5.104	61.348	1.00 39.87
	3668	CB	ILE	В	239	-9.165	-6.492	61.642	1.00 35.32
	3669	CG2	ILE	В	239	-8.936	-7.420	60.475	1.00 34.94
20	3670	CG1	ILE	В	239	-8.528	-7.092	62.886	1.00 32.97
	3671	CD1	ILE	В	23.9	-9.005	-8.480	63.222	1.00 31.96
	3672	С	ILE	В	239	-9.272	-4.511	60.148	1.00 42.94
	.3673	. 0	ILE	В	239	-8.857	-4.682.	59.004	1.00 43.05
	3674	N	LEU	В	240	-10.358	-3.802	60.437	1.00 80.50
25	3675	CA	LEU	В	240	-11.155	-3.148	59.417	1.00 83.41
	3676	CB	LEU	В	240	-12.435	-2.583	60.025	1.00108.88
	3677	CG	LEU	В	240	-13.154	-1.558	59.145	1.00110.23
	3678	CD1	LEU	В	240	-13.680	-2.234	57.881	1.00109.99
	3679	CD2	LEU	В	240	-14.283	-0.912	59.936	1.00110.96
30	3680	С	LEU	В	240	-10.350	-2.011	58.816	1.00 85.14
	3681	0	LEU	В	240	-9.800			1.00 86.33
	3682	N			241	-10.285	-0.901		1.00 88.35
	3683	CA	ALA	В	241	-9.556			1.00 88.88
	3684	СВ	ALA	В	241	-9.279	1.206	60.227	1.00 57.91
35	3685	С	ALA	В	241		-0.186		1.00 89.35
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	3688	CA	TYR	В	242	-6.430	-1.760		1.00 69.38
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40	3690	CG			242	-5.017	-3.847	58.243	1.00 59.73
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	3693	CD2	TYR	В	242	-5.224	-5.164	57.838	1.00 58.12

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       3707
             N
                 ARG B 244
                                 -9.109
                                          -0.701
                                                  55.199
                                                           1.00 64.72
 15
       3708
             CA
                 ARG B 244
                                 -9.594
                                           0.540
                                                  54.611
                                                           1.00 67.47
       3709
                 ARG B 244
             CB
                                -10.226
                                           1.424
                                                  55.681
                                                           1.00 94.83
       3710
             CG
                 ARG B 244
                                -11.040
                                           2.574
                                                  55.119
                                                           1.00 96.30
      3711
             CD
                 ARG B 244
                                -12.422
                                           2.113
                                                  54.689
                                                           1.00 98.16
      3712
             NE
                 ARG B 244
                                -13.377
                                           2.045
                                                  55.803
                                                          1.00 99.54
 20
      3713
             CZ
                 ARG B 244
                                -13.363
                                           1.139
                                                  56.781
                                                          1.00 99.23
      3714
            NH1 ARG B 244
                                -12.436
                                          0.191
                                                  56.810
                                                          1.00 99.50
      3715
            NH2 ARG B 244
                                -14.286
                                          1.181
                                                  57.734
                                                          1.00 98.66
      3716
            С
                 ARG B 244
                                 -8.435
                                          1.290
                                                  53.961
                                                          1.00 69.17
      3717
                 ARG B 244
            0
                               -8.625
                                          2.043
                                                  53.006
                                                          1.00 69.16
25
      3718
            Ν
                 ARG B 245
                                 -7.231
                                          1.078
                                                  54.483
                                                          1.00 90.19
      3719
                 ARG B 245
            CA
                                 -6.046
                                          1.746
                                                  53.960
                                                          1.00 92.43
      3720
            CB
                ARG B 245
                                 -4.814
                                          1.401
                                                  54.805
                                                          1.00 79.40
      3721
            CG
                ARG B 245
                                -5.013
                                          1.508
                                                 56.315
                                                          1.00 78.40
      3722
            CD
                ARG B 245
                                -5.394
                                          2.918
                                                 56.755
                                                          1.00 78.14
30
      3723
            NE
                ARG B 245
                                -5.540
                                          3.030
                                                 58.208
                                                          1.00 77.20
      3724
            CZ
                ARG B 245
                                -4.539
                                          2.903
                                                 59.078
                                                          1.00 76.66
     3725
            NH1 ARG B 245
                                -3.306
                                          2.658
                                                 58.650
                                                          1.00 76.13
     3726
            NH2 ARG B 245
                                -4.771
                                          3.019
                                                 60.379
                                                          1.00 75.87
     3727
            С
                ARG B 245
                                -5.791
                                          1.326
                                                 52.522
                                                          1.00 94.57
35
     3728
            0
                ARG B 245
                                -5.595
                                          0.147
                                                 52.235
                                                          1.00 94.29
     3729
           N
                HIS B 246
                                -5.813
                                          2.293
                                                 51.617
                                                          1.00142.27
     3730
           CA
                HIS B 246
                                -5.547
                                          2.018
                                                 50.213
                                                         1.00144.64
     3731
           CB
                HIS B 246
                                -6.640
                                          2.603
                                                 49.304
                                                         1.00124.13
     3732
           CG
                HIS B 246
                                -8.010
                                         2.052
                                                 49.544
                                                         1.00125.01
40
           CD2 HIS B 246
     3733
                                -9.171
                                         2.669
                                                 49.869
                                                         1.00125.08
     3734
           ND1 HIS B 246
                                -8.313
                                         0.715
                                                 49.402
                                                         1.00125.24
     3735
           CE1 HIS B 246
                                -9.602
                                         0.532
                                                 49.627
                                                         1.00125.20
     3736
           NE2 HIS B 246
                               -10.145
                                         1.702
                                                 49.912
                                                         1.00125.75
```

	3737	. С	HIS B	246		-4.250	2.744	49.899	1.00	0145.61
	3738	0	HIS B	246		-3.154	2.346	50.307		0146.34
	3739	N	ARG B	247		-4.434	3.837	49.171		74.46
	3740	CA	ARG B	247		-3.401	4.755	48.712	1.00	74.85
5	3741	СВ	ARG B	247		-2.260	4.001	48.003	1.00	74.20
	3742	CG	ARG B	247		-2.692	2.816	47.140	1.00	72.35
	3743	CD	ARG B	247		-1.503	1.878	46.868	1.00	71.58
	3744	NE	ARG B	247	,	-1.904	0.644	46.187	1.00	70.02
	3745	CZ	ARG B	247		-2.762	-0.249	46.681	1.00	69.37
10	3746	NH:	l ARG B	247		-3.322	-0.059	47.871	1.00	69.43
	3747	NH	2 ARG B	247	•	-3.075	-1.331	45.976	1.00	67.98
	3748	С	ARG B	247		-4.187	5.644	47.750	1.00	75.12
	3749	0	ARG B	247	•	-3.634	6.502	47.058	1.00	74.84
	3750	N	ARG B	248	-	-5.505	5.424	47.755	1.00	75.10
15	3751	CA	ARG B	248	•	-6.450	6.146	46.914	1.00	74.94
	3752	CB	ARG B	248	-	-6.517	7.627	47.328	1.00	73.91
	3753	CG	ARG B	248	-	-7.534	8.433	46.515	1.00	72.01
	3754	CD	ARG B		-	-7.514	9.937	46.808	1.00	69.76
20	3755	NE	ARG B			-8.134		45.719	1.00	67.75
20	3756	CZ	ARG B			-9.384			1.00	67.22
	3757		ARG B				9.633	45.832	1.00	66.89
	3758		ARG B			9.827				65.91
	3759	С	ARG B			6.053	•	45.437	1.00	75.28
25	3760	0	ARG B			5.857		44.719		75.09
25	3761	N	PHE B				4.758			75.96
	3762	CA	PHE B				4.469			76.80
	3763	CB	PHE B			4.998		43.499		76.98
	3764	CG	PHE B				2.031			
30	3765		PHE B				1.945			
50	3766		PHE B			5.027	1.177	45.203		
	3767		PHE B			7.810	1.024			77.84
	3768		PHE B			5.698		46.008		77.54
	3769 3770	CZ C	PHE B 2			7.093	0.173	45.968		77.55
35	3771	0	PHE B 2			6.722	4.658	42.614		77.29
33	3772	OT	PHE B 2			7.013	3.708	41.838		77.59
	3773		IPP C	1		7.325	5.763	42.625		77.59
	3774		IPP C	1		3.752	-1.490	77.726		33.83
	3775		IPP C	1		2.891	-0.835	78.560		33.83
40	3776		IPP C	1		4.416	-2.798	78.081		33.83
.0	3777		IPP C	1		4.097 5.075	-0.941	76.373		33.83
	3778		IPP C	1			0.215 3.852	76.421		33.83
	3779		IPP C	1				77.104		33.83
	3.73		-11 C	-	4	1.021	2.417	77.787	1.00	33.83

	WO 03/0)48733					PCT	/US02/38715
	3780	O16 IPP C	1	6.225	2.006	78.323	1.00 33.83	
	3781	O17 IPP C	1	4.317	1.406	76.629	1.00 33.83	
	3782	O18 IPP C	1 '	, 3.695	2.471	78.827	1.00 33.83	
	3783	P19 IPP C	1	5.684	5.144	77.406	1.00 33.83	'
5	3784	O20 IPP C	. 1	7.110	4.945	76.880	1.00 33.83	1
	3785	O21 IPP C	1	4.994	6.358	76.768	1.00 33.83	ı
	3786	O22 IPP C	1	5.646	5.185	78.935	1.00 33.83	
	3787	CO1 IPP C	2	2.307	-3.138	81.526	1.00 33.83	
•	3788	CO2 IPP C	2 ,	3.668	-3.126	81.578	1.00 33.83	•
10	3789	CO5 IPP C	2	1.513	-4.452	81.609	1.00 33.83	
	3790	CO9 IPP C	2	1.487	-1.841	81.385	1.00 33.83	
	3791	C12 IPP C	2 .	1.887	-0.699	82.354	1.00 33.83	
	3792	O14 IPP C	2	-0.767	2.198	82.197	1.00 33.83	
	3793	P15 IPP C	2	0.246	1.188	81.498	1.00 33.83	,
15	3794	O16 IPP C	2 .	-0.425	0.460	80.333	1.00 33.83	÷
	3795	O17 IPP C	2	0.736	0.134	82.638	1.00 33.83	
	3796	O18 IPP C	2	1.498	2.051	81.154	1.00 33.83	•
	3797	P19 IPP C	2	-1.027	3.757	81.972	1.00 33.83	
	3798	O20 IPP C	2	-0.542	4.097	80.558	1.00 33.83	
20	3799	O21 IPP C	2	-2.512	4.040	82.143	1.00 33.83	
	3800	O22 IPP C	2	-0.165	4.429	83.060	1.00 33.83	
	3801	OH2 WAT W	1	12.965	-11.206	62.097	1.00 33.83	
	3802	OH2 WAT W	2	11.962	-27.690	81.314	1.00 33.83	
_	3803	OH2 WAT W	3	2.139	4.914	· 78 · 332 ·	1.00 33.83	rene e e e e e e
25	3804	OH2 WAT W	4		-9.399		1.00 33.83	
	3805	OH2 WAT W	5 [12.062	14.669	72.584	1.00 33.83	1

END

Table IIA. Interatomic distances in the native UPPS structure

	i able i	IA. IIILEI al	onnic dista	11069 111	uie nauve or	ro structu	re
٠	FROM TO	DIS	TANCE,		27CE	71N	3.956
	•	A	ngstrom	45	27C	270	1.230
5	27N	27CA	1.470		27C	28N	1.328
	27N	27CB	2.442		27C	27CA	1.515
	27N	27C	2.480		27C	28CA	2.451
	27N	27CG	2.947		27C	27N	2.480
	27N	28N	3.122	50	27C	27CB	2.501
10	27N	700	3.142	ţ	27C	28C	3.406
	27N	270	3.285		27C	28CB	3.563
	27CA	27N	1.470		27C	280	3.753
	27CA	27C	1.515		27C	27CG	3.873
	27CA	27CB	1.531	55	270	27C	1.230
15	27CA	270	2.394		270	28N	2.255
	27CA	28N	2.404		270	27CA	2.394
	27CA	27CG	2.545		270	27CB	2.749
	27CA	28CA	3.793		270	28CA	2.816
	27CA	700	3.988	60	270	27N	3.285
20	27CB	27CG	1.526		270	72N	3.332
	27CB	27CA	1.531		270	72CA	3.576
	27CB	27N	2.442		270	28C	3.674
1	. 27CB	27C	2.501	e ^c	270	72CB	3.836
	27CB	270	2.749	65	. 28N	27C	1.328
25	27CB	27SD	2.828		28 N	28CA	1.456
	27CB	27CE	3.129		28N	270	2.255
	27CB	28N	3.678		28N	28CB	2.396
	27CB	700	3.850		28N	27CA	2.404
	27CG	27CB	1.526	70	28N	28C	2.490
30	27CG	27SD	1.817		28N	280	2.808
	27CG	27CA	2.545		28N	27N	3.122
	27CG	27CE	2.831		28N	28CG	3.615
	27CG	27N	2.947		28N	29N	3.640
	27CG	27C	3.873	75	28N	27CB	3.678
35	27SD	27CG	1.817	•	28CA	28N	1.456
	27SD	27CE	1.863		28CA	28CB	1.524
	27SD	27CB	2.828		28CA	28C	1.546
	27CE	27SD	1.863		28CA	280	2.410
	27CE	27CG	2.831	80	28CA	27C	2.451
40	27CE	27CB	3.129		28CA	29N	2.466
	27CE	700	3.804		28CA	28CG	2.518
	27CE	71CA	3.877		28CA	270	2.816
	27CE	70C	3.929		28CA	280D1	3.045
	•			400			

	WO 03/048733					PC	CT/US02/38715
	28CA	280D2	3.384		28C	27C	3.406
	28CA	27CA	3.793	45	28C	28CG	3.411
	28CA	29CA	3.824		28C	280D1	3.456
	28CA	72CD1	3.860		28C	29C	3.518
5	28CB	28CG	1.490		28C	270	3.674
	28CB	28CA	1.524		' 28C	30N	3.732
	28CB	280D2	2.338	50	280	28C	1.228
	28CB	280D1	2.356		280	29N	2.239
	28CB	28N	2.396		280	28CA	2.410
10	28CB	28C	2.500		280	29CA	2.711
	28CB	280	3.169		280	28N	2.808
	28CB	29N	3.287	55	280	28CB	3.169
	28CB	27C	3.563	•	280	29C	3.724
	28CG	280D1	1.240		280	2,7C	3.753
15	28CG	280D2	1.244		29N	28C	1.331
	28CG	28CB	1.490	.,	29N	29CA	1.458
	28CG	28CA	2.518	60	29N	280	2.239
	28CG	72CD1	3.356	•	29N	28CA	2.466
	28CG	28C	3.411		29N	29C	2.585
20	28CG	72CE1	3.411		29N	30N	2.897
	28CG	28N	3.615		29N	28CB	3.287
	28CG	29N	3.697	.65	29N	280D1	3.296
	280D1	28CG	1.240		29N	28N	3.640
	280D1	280D2	2.190	a ,	29N	290	3.691
25	28OD1	28CB	2.356	•	29N	28CG	3.697
	28OD1	72CE1	2.694		29CA	29N	1.458
	280D1	28CA	3.045	70	29CA	29C	1.520
	280D1'	72CD1	3.057		29 <u>C</u> A	290	2.380
	280D1	29N	3.296		29CA	28C .	2.410
30	280D1	28C	3.456		29CA	30N	2.454
	280D1	72CZ	3.710		29CA	280	2.711
	280D2	28CG	1.244	75	29CA	30CA	3.802
	280D2	280D1	2.190		29CA	28CA	3.824
	280D2	28CB	2.338		29C	290	1.234
35	280D2	28CA	3.384		29C	30N	1.333
	280D2	72CD1	3.624		29C	29CA	1.520
	280D2	72CE1	3.724	80	29C	30CA	2.408
٠	28C	280	1.228		29C	29N	2.585
	28C	29N	1.331		29C	30C	2.963
40	28C	28CA	1.546	•	29C	31N	3.163
	28C	29CA	2.410		29C	28C	3.518
	28C	28N	2.490	85	29C	30CB	3.696
	28C	28CB	2.500		29C	280	3.724

•	WO 03/048733					PC	CT/US02/38715
	29C	30ND2	3.761		30CB	300	3.224
	29C	300	3.854	45	30CB	45CD2	3.655
	290	29C	1.234		30CB	29C	3.696
	290	30N	2.247		30CG	300D1	1.229
5	290	29CA	2.380		30CG	30ND2	1.311
	290	30CA	2.717		30¢G	30CB	1.496
	290	30C	2.845	50	30CG	30CA	2.502
-	290	31N	3.224		30CG	30N	2.971
	290	300	3.391		30CG	30C	3.825
10	290	, 32N	3.461		30CG	45CD2	3.961
	290	29N	3.691		300D1	30CG	1.229
	290	32C	3.973	55 ,	. 300D1	30ND2	2.230
	30N	29C	1.333		300D1	30CB	2.380
	30N	30CA	1.452		300D1	45CD2	3.392
15	30N	290	2.247		300D1	30CA	3.656
	30N	30CB	2.444		300D1	45CA	3.772
	30N	29CA	2.454	60	30ND2	30CG	1.311
	30N	30C	2.470		30ND2	300D1	2.230
	30N	30ND2	2.764		30ND2	30CB	2.380
20	30N	31N	2.805		30ND2	30CA	2.652
*	. 30N	29N	2.897		30ND2	30N	2.764
	30N	30CG	2.971	65	30ND2	29C	3.761
	, 30N	300	3.526		. ; 30C,	300	1.229
•	30и	28C	3.732		30C	31N	1.336
25	30CA	30N	1.452		30C.	30CA	1.527
	30CA	30CB	1.518		30C	31CA	2.435
	30CA	30C	1.527	70	30C	30N	2.470
	30CA	300	2.391		30C	30CB	2.480
	30CA	29C	2.408		30C	290	2.845
30	30CA	31N	2.442		30C	29C	2.963
	30CA	30CG	2.502		30C	31C	3.116
	30CA	30ND2	2.652	75	30C	32N	3.583
	30CA	290	2.717		30C	30CG	3.825
	30CA	300D1	3.656		30C	310	3.839
35	30CA	29CA	3.802		300	30C	1.229
	30CA	31CA	3.812		300	31N	2.256
	30CB	30CG	1.496	80	300	30CA	2.391
	30CB	30CA	1.518		300	31CA	2.775
	30CB	300D1	2.380		300	31C	3.111
40	30CB	30ND2	2.380		300	30CB	3.224
	30СВ	30N	2.444		300	290	3.391
	30CB	30C	2.480	85	300	310	3.441
	30CB	31N	3.172		300	30N	3.526

WO	03/048733					PC	T/US02/38715
	300	32N	3.804		32N	31CA	2.431
	300	29C	3.854	45	32N	32C	2.438
•	31N	30C	1.336		32N	32CB	2.466
	31N	31CA	1.454		32N	31N	2.938
5	31N	300	2.256		32N	32CG	3.309
	31N	30CA	2.442		32N	290	3.461
	31N	31C	2.491	50	32N	320	3.504
	31N	30N	2.805		32N	30C	3.583
	31N	32N	2.938		32N	300	3.804
10	31N	29C	3.163		32CA	32N	1.457
	31N	30CB	3.172		32CA	32C	1.531
	31N	290	3.224	55	32CA	32CB	1.534
	31N	310	3.471		32CA	320	2.397
	31CA	31N	1.454		32CA	31C	2.434
15	31CA	31C	1.515		32CA	32CG	2.585
	31CA	310	2.378		32CA	310	2.775
	31CA	32N	2.431	60	32CA	31CA	3.803
	31CA	30C	2.435		32CA	32CD	3.927
	31CA	300	2.775		32CB	32CG	1.531
20	31CA	32CA	3.803		32CB	32CA	1.534
	31CA	30CA	3.812		32CB	32N	2.466
	31C	310	1.230	65	32CB	32C	2.495
	31C	32N	1.331		32CB	32CD	2.539
	31C	31CA	1.515	."	32CB	32NE	3.067
25	31C	32CA	2.434		. 32CB	320	3.244
•	31C	31N	2.491		32CB	31C	3.727
	31C	32C	2.939	70	32CG	32CB	1.531
	31C	300	3.111		32CG	32CD	1.535
	31C	30C	3.116		32CG	32NE	2.519
30	31C	32CB	3.727		32CG	32CA	2.585
	31C	320	3.847		32CG	32N	3.309
	310	31C	1.230	75	32CG	32CZ	3.766
	310	32Ņ	2.253		32CG	32C	3.838
	310	31CA	2.378		32CD	32NE	1.467
35	310	32CA	2.775		32CD	32CG	1.535
	310	32C	2.870		32CD	32CZ	2.476
	310	320	3.433	80	32CD	32CB	2.539
	310	300	3.441		32CD	32NH1	2.829
	310	31N ,	3.471		32CD	32NH2	3.686
40	310	30C	3.839		32CD	32CA	3.927
	32N	31C	1.331		32NE	32CZ	1.336
	32N	32CA	1.457	85	32NE	32CD	1.467
	32N	310	2.253		32NE	32NH1	2.311

W	0 03/048733		·			PCT	T/US02/38715
	32NE	32NH2	2.314		45CA	45ND1	3.589
	32NE	32CG	2.519	45	45CA	300D1	3.772
	32NE	32CB	3.067		45CB	45CG	1.497
	32CZ	32NH2	1.329		45CB	45CA	1.532
5	32CZ	32NH1	1.329	•	45CB	45N	2.449
	32CZ	32NE	1.336		45CB	45ND1	2.527
	32CZ	32CD	2.476	50	45CB	45C	2.535
	32CZ	32CG	3.766		45CB	45CD2	2.596
	32NH1	32CZ	1.329		45CB	450	3.264
10	32NH1	32NH2	2.292		45CB	45CE1	3.631
	32NH1	32NE	2.311		45CB	45NE2	3.673
	32NH1	32CD	2.829	55	45CG	45CD2	1.356
	32NH2	32CZ	1.329		45CG	45ND1	1.379
	32NH2	32NH1	2.292		45CG	45CB	1.497
15	32NH2	32NE	2.314		45CG	45NE2	2.200
	32NH2	32CD	3.686		45CG	45CE1	2.206
	32C	320	1.226	60	45CG	45CA	2.520
	32C	32CA	1.531		45CG	45N	2.975
	32C	32N	2.438		45CG	45C	3.865
20	32C	32CB	2.495		45CD2	45CG.	1.356
	32C	310	2.870		45CD2	45NE2	1.376
	32C	31C	2.939	65	45CD2	45ND1	2.185
	32C	32CG	3.838		45CD2	45CE1	2.195
	32C	290	3.973		45CD2	45CB	2.596
· 25	320	32C	1.226		45CD2	45CA	3.208
	320	32CA	2.397		45CD2	300D1	3.392
	320	32CB	3.244	70	45CD2	30CB	3.655
	320	310	3.433		45CD2	45N	3.660
	320	32N	3.504		45CD2	30CG	3.961
30	320	31C	3.847		45ND1	45CE1	1.322
	45N	45CA	1.457		45ND1	45CG	1.379
	45N	45C		75	45ND1	45NE2	2.145
	45N	45CB	2.449		45ND1	45CD2	2.185
	45N	45CG	2.975		45ND1	45CB	2.527
35	45N	450	3.510		45ND1	45CA	3.589
	45N	45ND1	3.612		45ND1	45N	3.612
	45N	45CD2	3.660	80	45CE1	45NE2	1.322
	45CA	45N	1.457		45CE1	45ND1	1.322
	45CA	45C	1.515		45CE1	45CD2	2.195
40	45CA	45CB	1.532		45CE1	45CG	2.206
	45CA	450	2.382	0-	45CE1	45CB	3.631
	45CA	45CG	2.520	85	45NE2	45CE1	1.322
	45CA	45CD2	3.208		45NE2	45CD2	1.376

	WO 03/048733					PC	T/US02/38715
	45NE2	45ND1	2.145		480	49CA	2.787
	45NE2	45CG	2.200	45	480	52N	2.961
	45NE2	45CB	3.673	,	480	49C	2,992
	45C	450	1.219		480	48N	3.474
5	45C	45CA	1.515		480	490	3.497
	45C	45N	2.445		480	52CB	3.661
	45C	45CB	2.535	50	480	52CA	3.871
	45C	48N	3.564		49N	48C	1.339
	45C	45CG	3.865		49N	49CA	1.467
10	450	45C	1.219		49N	480	2.266
	450	45CA	2.382		49N	48CA	2.435
	450	49N	2.958	55	49N	49C	2.446
·	450	48N	3.126	•	49N	49CB	2.492
	450	45CB	3.264		49N	48N	2.721
15	450	45N	3.510		49N	450	2.958
	450	48CA	3.519		4 9N	49CG	3.422
	450	48C	3.661	60	4 9 N	490	3.509
	450	49CB	3.852		49CA	49N	1.467
	450	49CA	3.942		49CA	49C	1.533
20	48N	48CA	1.449		49CA	49CB	1.539
	48N	48C	2.409		49CA	490	2.409
	48N	4 9 N	2.721	65	49CA	48C	2.446
	48N	450	3.126		49CA	49CĢ	2.603
	48N	480	3.474	F *	49CA	480	2.787
25	48N	45C	3.564		49CA	48CA	3.814
	48CA	48N	1.449		49CA	450	3.942
	48CA	48C	1.513	70	49CB	49CG	1.527
	48CA	480	2.379		49CB	49CA	1.539
20	48CA	4 9 N	2.435		4 9CB	49N	2.492
30	48CA	450	3.519		4 9CB	49C	2.502
	48CA	49CA	3.814		49CB	49SD .	2.839
	48C	480	1.235	75	4 9CB	490	3.272
	48C	49N	1.339	*	49CB	49CE	3.332
25	48C	48CA	1.513		49CB	48C	3.755
35	48C	48N	2.409		4 9CB	450	3.852
	48C	49CA	2.446	00	4 9CG	49CB	1.527
	48C	49C	3.014	80	4 9CG	49SD	1.852
	48C	450	3.661		49CG	49CA	2.603
40	48C	49CB	3.755		4 9CG	49CE	2.722
40	48C	490	3.882		4 9CG	49N	3.422
	480	48C	1.235	0.5	49CG	49C	3.813
	480	49N	2.266	85	49SD	49CE	1.728
	480	48CA	2.379		49SD	49CG	1.852

wo	03/048733					P(CT/US02/3871
	49SD	49CB	2.839	٠.	52CB	52CD1	2.516
	49CE	49SD	1.728	45	52CB	52CD2	2.530
	49CE	49CG	2.722		52CB	520	3.325
	49CE	49CB	3.332		• • 52CB	490	3.590
5	49C	490	1.232		52CB	480	3.661
	49C	49CA	1.533	• •	52CG	52CD1	1.528
	49C	49N	2.446	50	52CG	52CD2	1.531
	49C	49CB	2.502		52CG	52CB	1.545
	49C	480	2.992	•	52CG	52CA	2.602
10	49C	. 48C	3.014	•	52CG	52C	3.070
	49C	52N	3.736		52CG	520	3.399
	49C	49CG	3.813	55,	. 52CG	52N	3.887
	490	49C	1.232		52CD1	52CG	1.528
•	490	49CA	2.409		52CD1	52CD2	2.502
15	490	49CB	3.272		52CD1	52CB	2.516
	490	52N	3.272		52CD1	52CA	3.017
	490	480	3.497	60	52CD1	. 520	3.563
	490	49N	3.509		52CD1	52C	3.612
	490	52CB	3.590		52CD2	52CG	1.531
20	490	52CA	3.712		52CD2	52CD1	2.502
	490	5.2C	3.774		52CD2	52CB	2.530
	490	48C	3:882	65	52CD2	52CA	3.936
	, 52N ,	52CA	1.462	, .	::	5.20 .	1.227
	52N	52C	2.431		52C	52CA	1.519
25	52N	52CB	2.493		52C	· 52N	2.431
	52N	480	2.961		, 52C	52CB	2.510
	52N	490	3.272	70	52C	52CG	3.070
	52N	520	3.446		52C	52CD1	3.612
	52N	49C	3.736		52C	490	3.774
30	52N	52CG	3.887		520	52C	1.227
	52CA	52N	1.462		520	52CA	2.385
	52CA	52C	1.519	75	520	52CB	3.325
	52CA	52CB	1.544	*	520	52CG	3.399
	52CA	520	2.385		520	52N	3.446
35	, 52CA	52CG	2.602		520	52CD1	3.563
	52CA	52CD1	3.017		70N	70CA	1.453
	52CA	490	3.712	80	70N	70CB	2.386
	52CA	480	3.871		70N	70C	2.439
	52CA	52CD2	3.936		70N	700	2.904
40	52CB	52CA	1.544		70N	71N	3.442
	52CB	52CG	1.545		70N	7,0CG	3.785
	52CB	52N	2.493	85	70CA	70N	1.453

70CA

1.517

70CB

2.510

52CB

52C

W	0 03/048733					PC	T/US02/3871
	70CA	70C	1.519		70CE1	70CD2	2.772
	70CA	700	2.393	45	70CE1	70CB	3.808
	70CA	71N	2.421		70CD2	70CE2	1.380
	70CA	70CG	2.582		70CD2	70CG	1.392
5	70CA	70CD1	3.068	1	70CD2	70CD1	2.387
	70CA	70CD2	3.793		70CD2	70CZ	2.394
	70CA	71CA	3.804	50	70CD2	70CB	2.510
	70CB	70CG	1.502		70CD2	70CE1	2.772
	70CB	70CA	1.517		70CD2	700H	3.639
10	70CB	70N	2.386		70CD2	70CA	3.793
	70CB	70C	2.487		70CE2	70CD2	1.380
	70CB	70CD2	2.510	55	70CE2	70CZ	1.385
	70CB	70CD1	2.521		70CE2	700H	2.380
	70CB	700	2.952		70CE2	70CE1	2.396
15	70CB	71N	3.466		70CE2	70CG	2.414
	70CB	70CE2	3.780		70CE2	70CD1	2.760
	70CB	70CE1	3.808	60	70CE2	70CB	3.780
	70CG	70CD1	1.391		70CZ	700H	1.367
	70CG	70CD2	1.392		70CZ	70CE1	1.376
20	70CG	70CB	1.502		70CZ	70CE2	1.385
	70CG	70CE2	2.414		70CZ	70CD1	2.394
	70CG	70CE1	2.432	65	70CZ	70CD2	2.394
	70CG	70CA	2.582		70CZ	70CG	2.791
	70CG	70CZ	2.791	2	700н	70CZ	1.367
25	70CG	70C	3.132		• 700н	70CE1	2.371
	70CG	700	3.664		700н	70CE2	2.380
	70CG	71N	3.713	70	700H	70CD2	3.639
	70CG	70N	3.785		700н	70CD1	3.644
	70CD1	70CG	1.391		70C	700	1.238
30	70CD1	70CE1	1.400		70C	71N	1.321
	70CD1	70CD2	2.387		70C	70CA	1.519
	70CD1	70CZ	2.394	75	70C	71CA	2.436
	70CD1	70CB	2.521		70C	70N	2.439
	70CD1	70CE2	2.760		70C	70CB	2.487
35	70CD1	70CA	3.068		70C	71C	3.127
	70CD1	70C	3.613		70C	70CG	3.132
	70CD1	700H	3.644	80	70C	72N	3.541
	70CD1	71N	3.740		70C	70CD1	3.613
	70CE1	70CZ	1.376		70C	71CB	3.684
40	70CE1	70CD1	1.400		70C	710	3.882
	70CE1	700H	2.371		70C	27CE	3.929
	70CE1	70CE2	2.396	85	700	70C	1.238
	70CE1	70CG	2.432		700	71N	2.251

wo	03/048733					PC	F/US02/3871:
	700	70CA	2.393		71C	72CA	2.475
	700	71CA	2.782	45	71C	71CB	2.505
	700	70N	2.904		71C.	71N	2.507
	700	70CB	2.952		71C	70C	3.127
5	700	72N	3.044	,	71C	700	. 3.133
	700	71C	3.133		71C	72CB	3.251
	700	27N	3.142	50	710	71C	1.236
	700	. 70CG	3.664	,	710	72N	2.274
	700	27CE	3.804		710	71CA	2.415
10	700	. 27CB	3.850		710	72CA	2.843
	700	27CA	3.988		710	71CB	2.849
	71N	70C	1.321	55 .	710	71N	3.137
	71N	71CA	1.462		710	72CB	3.448
·	71N	700	2.251		710	70C	3.882
15	71N	70CA	2.421		72N	· 71C	1.342
	71N ,	71CB	2.434		72N	72CA	1.470
	71N	71C	2.507	60	72N	710	2.274
	71N	710	3.137		72N	72CB	2.456
	71N	72N	3.354		72N	71CA	2.459
20	71N	70N.	3.442		72N	700	3.044
	71N	70 <u>C</u> B	3.466		72N	270	3.332
	71N	70CG	3.713	65	72N	71N	3.354
	. 71N	70CD1	3.740	, ,	72N	70C.	3.541
	71N	27CE	3.956		72N	71CB	3.608
25	71CA	71N	1.462		72N	72CG	3.820
	71CA	71CB	1.517		72CA	72N	1.470
	71CA	71C	1.549	70	72CA	72CB	1.536
1	71CA	710	2.415		72CA	71C	2.475
	71CA	70C	2.436		72CA	72CG	2.554
30	71CA	72N	2.459		72CA	710	2.843
	71CA	700	2.782		72CA	72CD2	3.379
	71CA	70CA	3.804	75	72CA	72CD1	3.398
	71CA	72CA	3.860		72CA	270	3.576
	71CA	27CE	. 3.877		72CA	71CA	3.860
35	71CB	71CA	1.517		72CB	72CG	1.507
	71CB	71N	2.434		72CB	72CA	1.536
	71CB	71C	2.505	80	72CB	72N	2.456
	71CB	710	2.849		72CB	72CD2	2.513
	71CB	72N	3.608		72CB	72CD1	2.518
40	71CB	70C	3.684		72CB	71C	3.251
	71C	710	1.236		72CB	710	3.448
	71C	72N	1.342	85	72CB	72CE2	3.802
	71C	71CA	1.549		72CB	72CE1	3.806

w	03/048733					PC	T/US02/38715
	72CB	270	3.836		72CZ	72CE1	1.384
	72CG	72CD2	1.387	45	72CZ	72CD2	2.406
	72CG	72CD1	1.388		72CZ	72CD1	2.410
•	72CG	72CB	1.507		72CZ	72CG	2.799
5	72CG	72CE2	2.420		72CZ	280D1	3.710
	72CG	72CE1	2.421		72C	72CA	1.526
	72CG	72CA	2.554	50	72C	72N	2.477
	72CG	72CZ	2.799		72C	72CB	2.499
	72CG	72N	3.820		72C	710	2.651
10	72CD1	72CG	1.388		72C	71C	2.881
	72CD1	72CE1	1.398		72C	72CG	3.042
	72CD1	72CD2	2.388	55	72C	72CD2	3.243
	72CD1	72CZ	2.410		720	72CA	2.410
	72CD1	72CB	2.518		720	72CB	3.415
15	72CD1	72CE2	2.769		720	72N	3.450
	72CD1	280D1	3.057		720	72CG	3.541
	72CD1	28CG	3.356	60	['] 720	72CD2	3.581
	72CD1	72CA	3.398		720	710	3.734
	72CD1	28OD2	3.624		720	71C	3.950
20	72CD1	28CA	3.860		90CD1	45CB	3.755
	72CD2	72CG	1.387		90CD2	49CE	3.288
	72CD2	72CE2	1.396	65	900	49SD	3.899
4	72CD2	72CD1	2.388		94N	49SD	3.988
	72CD2	72CZ	2.406	<i></i>	94CA	49SD	3.982
25	72CD2	72CB	2.513		143CE2	52CD2	3.572
,	72CD2	72CE1	2.767		143CZ	52CD2	3.734
	72CD2	72CA	3.379	70	200NE	280D2	3.552
	72CE1	72CZ	1.384		200CZ	280D2	3.594
	72CE1	72CD1	1.398		200NH2	280D2	2.807
30	72CE1	72CE2	2.392		200NH2	28CG	3.947
	72CE1	72CG	2.421		2080	70CE2	3.609
	72CE1	280D1	2.694	75	2080	700H	3.637
	72CE1	72CD2	2.767				
25	72CE1	28CG	3.411				
35	72CE1	280D2	3.724				
	72CE1	72CB	3.806		•	•	
	72CE2	72CZ	1.381				v.
	72CE2	72CD2	1.396				
40	72CE2	72CE1	2.392				
+∪	72CE2 72CE2	72CG	2.420				
		72CD1	2.769	•			
	72CE2	72CB 72CE2	3.802			,	
	72CZ	IZCEZ	1.381				

					101A	79NH1	3.816
	Table IIB				101A	31N	3.871
	Interatomic dis	tances in	the active	45	102A	79NH2	3.383
	site of UPPS ir				102A	280D2	3.815
5	FROM	то	***************************************		103A	29N	3.119
	DISTANCE, Ang				103A	30N	3.133
	1C1	79NH1	3.600	•	103A	31N	3.539
	1C1	79NH2	3.700	50	103A	29C	3.628
	101	270	3.689		103A	30CB	3.710
10	1C2	300D1	3.734		103A	29CA	3.773
	1C2	45NE2	3.829		103A	30CA	3.821
	1C2	79NH1	3.943		1PB	29N	3.332
	1C3	710	3.693	55	1PB	29CA	3.751
	1C4	710	3.205		1PB	29C	3.892
15	1C4	71C	3.901		1PB	30N	3.917
	1C5	710	3.250		1PB	31N	3.953
•	1C5	45CD2	3.935		101B	280D2	3.279
	1C6	300D1	3.590	60	101B	29N	3.303
	1C6	710	3.792		101B	28CG	3.959
20	1C7	710	3.815		103B	29CA	3.054
	1C10	49N	3.149		103B	32N	3.066
	1C10	450	3.182	<i>c =</i>	103B	32CB	3.174
,	1C10	48C	3.455	65	103B	29¢	3.179
	1C10	48CA	3.529		103B	29N	3.239
25	1C10	300D1	3.732		103B	290	3.525
٠	1C10	49CA	3.898		103B	30N	3.683
"	1C11	90CD1	3.926	70	103B	31N	3.695
	1C13	143CE2	3.797	70	103B	32CA	3.724
	1C14	143CE2	3.506		·		
30 .	1C14	143CZ	3.626				
	1C14	143CD2	3.943				
	1C14	91CG	3.966				
	1C14	91CA	3.973				
	1C15	49SD	3.501				
35	1C15	94CG	3.603				
	1C15	94CB	3.631		•		
	1C15	94CD1	3.657				e ²
	1C15	49CG	3.786				
40	1C15	900	3.878				
40	1PA	79NH2	3.866				
	101A	79NH2	3.513		•		
	101A	45CE1	3.716				

•	WO 03/048733					PCT/US02/3871		
		·			1017	28OD2	3.512	
	Table IIC. Inte	ratomic dis	tances in	35	, 1017	28CG	3.928	
	the active site	of UPPS in	n complex		1018	28OD2	2.364	
	with IPP		•		1018	28CG	3.315	
5	FROM	то			1018	247NH2	3.318	
	DISTANCE, And				1018	280D1	3.896	
	1C01	700	3.809	40	1P19	2080G	3.381	
	1C02	280D2	3.216		1P19	250CA	3.746	
	1C02	270	3.687		1P19	206NH1	3.934	
10	1C02	28CB	3.980		1P19	2470	3.982	
	1C05	710	2.963		1P19	206CD	3.996	
	1C05	700	3.179	45	1020	2080G	2.922	
	1C05	71C	3.316	1	1020	250N	3.251	
	1C05	72N	3.740		1020	250CA	3.346	
15	1C05	70C	3.796		1020	217CE2	3.424	
	1C05	72CA	3.902		1020	208CB	3.573	
•	1C05	76ND2	3.926	50	1020	2470	3.929	
	1C09	70CD2	3.339		1021	206NH1	2.419	
	1C09	70CE2	3.717		1021	206CD	2.885	
20	1C09	70CG	3.726		1021	206CZ	3.136	
	1C12	70CE2	3.543		1021	206NE	3.301	
	1C12	70CD2	3.700	55	1021	2080G	3.619	
	1014	200NH2	3.012		1021	200NH2	3.888	
	1014	2080G	3.176	1.1	1022	250CA	2.964	
25	1014	208CB	3.901		1022	247NE	3.080	
	1P15 .	280D2	3.515		1022	2470	3.568	

247CZ

247CG

247CD

250N

2500

247NH2

250C

3.603

3.609

3.669

3.708

3.789

3.794

3.945

70

30

1P15

1016

1016

1016

1016

1016

1017

200NH2

76ND2

760D1

76CG

250CA

730G

200NH2

3.515

3.785

3.221

3.395

3.703

3.833

3.895

3.277

60

65

1022

1022

1022

1022

1022

1022

1022

Table IIIA Interatomic angle between residues in the active site of the native UPPS

	ATOM1	ATOM2	ATOM3	ANGLE, degree
	27CA	27N	27CB	36.380
75	27CA	27N	27C	34.390

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WO 03/048733				PCT/US02/38715
27CA	27N	27CG	59.730	
		0.017	40 110	

	27CA	27N	27CG	59.730
	27CA	27N	28N	48.110
•	27CA	27N	700	114.81
	27CA	27N	270	41.610
5	27CB	27N	27C	61.060
	27CB	27N	27CG	31.140
	27CB	27N	28N	81.760
	27CB	27N	700	86.200
	27CB	27N	270	55.020
10	27C	, 27N	27CG	90.640
	27C	27N	28N	24.120
	27C	27N	700	105.55
	27C	27N	270	18.750
	27CG	27N	28N	107.82
15	27CG	. 27N	700	86.660
	27CG ,	27N	270	86.150
	28N	27N	700	122.16
	28N	27N	270	41.130
	700	27N	270	87.110
20	27 n	27CA	27C	112.36
	27N	27CA	27CB	108.92
	27N	27CA	270	114.32
•	2.7N	27CA	, 28N	104.81
	27N	27CA	27CG	90.350
25	27N	27CA	28CA	106.75
•	27N .	27CA	700	45.650
	27C	27CA	27CB	110.35
	27C	27CA	270	26.110
	27C	27CA	28N	29.970
30	27C	27CA	27CG	143.84
	27C	27CA	28CA	21.730
	27C	27CA	700	99.510
	27CB	27CA	270	85.940
	27CB	27CA	28N	137.21
35	27CB	27CA	27CG	33.580
	27CB	27CA	28CA	130.36
	27CB	27CA	700	73.670
	270	27CA	28N	56.090
1	270	27CA	27CG	119.32
40	270	27CA	28CA	47.840
	270	27CA	700	83.930
	28N	27CA	27CG	164.74
	28N	27CA	28CA	8.280
	•			420

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	28N	27CA	700	115.89
	27CG	27CA	28CA	161.71
	27CG	27CA	700	76.000
	28CA	27CA	700	111.21
5	27CG	27CB	27CA	112.71
	27CG	27CB	27N	93.000
	27CG	27CB	27C	147.22
	27CG	27CB	270	171.19
	27CG	. 27CB	27SD	35.510
.10	27CG	27CB	27CE	64.550
	27CG	27CB	28N	136.98
	27CG	27CB	700	91.600
	27CA	27CB	27N	34.700
	27CA	27CB	27C	34.610
15	27CA	27CB	270	60.300
	27CA	27CB	27SD	147.93
	27CA	27CB	27CE	148.37
	27CA	27CB	28N	26.360
	27CA	27CB	700	83.880
20	27N	27CB	27C	60.210
	27N	27CB	270	78.260
	27N	27CB	27SD	121.10
	27N	27CB	27CE	114.61
	27N	27CB	28N	57.150
25 .	27N	27CB	700	54.530
	27C	27CB	270	26.560
	27C	27CB	27SD	177.03
	27C	27CB	27CE	141.31
	27C	27CB	28N	11.650
30	27C	27CB	700	87.400
	270	27CB	27SD	150.53
•	270	27CB	27CE	118.05
	270	27CB	28N	37.710
	270	27CB	700	82.510
35	27SD	27CB	27CE	36.000
	27SD	27CB	28N	171.28
	27SD	27CB	700	91.440
	27CE	27CB	28N	152.38
	27CE	27CB	700	65.120
40	28N	27CB	700	93.470
	27CB	27CG	27SD	115.29
	27CB	27CG	27CA	33.710
	27CB	27CG	27CE	86.330
				421

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	27CB	27CG	27N	55.860
	27CB	27CG	27C	20.460
	27SD	27CG	27CA	148.72
	27SD	27CG	27CE	40.300
5	27SD	27CG	27N	148.35
	27SD	27CG	27C	135.74
	27CA	27CG	27CE	113.74
	27CA	27CG	27N	29.920
	27CA	27CG	27C	13.340
10	27CE	27CG	27N	108.96
	27CE	27CG	27C	103.84
	27N	27CG	27C	39.820
	27CG	27SD	27CE	100.58
	27CG	27SD	27CB	29.200
15	27CE	27SD	27CB	80.830
	27SD	27CE	27CG	39.120
	27SD	27CE	27CB	63.170
	27SD	27CE	700	112.50
	27SD	27CE	71CA	151.28
20	27SD	27CE	70C	125.18
	27SD	27CE	71N	144.45
	27CG	27CE	27CB	29.120
•	27CG	27CE	700	76.540
	27CG	27CE	71CA	112.15
25	27CG	27CE	70C	92.940
	27CG	27CE	71N	110.19
	27CB	27CE	700	66.630
	27CB	27CE	71CA	89.780
	27CB	27CE	70C	84.950
30	27CB	27CE	71N	96.340
	700	27CE	71CA	42.450
	700	27CE	70C	18.330
	700	27CE	71N	33.650
	71CA	27CE	70C	36.360
35	71CA	. 27CE	71N	21.480
	70C	27CE	71N	19.290
	270	27C	28N	123.65
	270	27C	27CA	121.05
	270	27C	28CA	93.890
40	270	27C	27N	120.82
	270	27C	27CB	88.040
	270	27C	28C	92.660
	270	27C	28CB	106.86
				422
				•

WO 03/0	48733					PCT/US02/38715
	270	٠.	27C	280	106.26	

	270	27C	280	106.26
	270	27C	27CG	100.06
	28N	27C	27CA	115.29
	28N	27C	28CA	29.780
5	28N	27C	27N	106.14
	28N	27C	27CB	146.02
	28N	27C	28C	37.660
	28N	27C	28CB	22.870
	28N	27C	280	36.990
10	28N	27C	27CG	135.19
	27CA	27C	28CA	145.05
	27CA	27C	27N	33.240
	27CA	27C	27CB	35.040
	27CA	27C	28C	139.44
15	27CA	27C:	28CB	129.53
	27CA	27C	280	120.75
	27CA	27C	27CG	22.820
	28CA	27C	27N	128.73
•	28CA	27C	27CB	168.13
20	28CA	27C	28C	24.300
	28CA	27C	28ÇB	20.290
	28CA	27C	280	39.070
	28CA	27C	27CG	163.41
	27N	27C	27CB	58.730
25	27N	27C	28C	143.49
	27N	27C	28CB	108.49
	27N	27C	280	132.89
	27N	. 27C	27CG	49.540
	27CB	27C	28C	143.99
30	27CB .	27C	28CB	164.54
	27CB	27C	280	129.27
	27CB	27C	27CG	12.320
	28C	27C	28CB	41.960
	28C	27C	280	18.970
35	28C	27C	27CG	144.47
	28CB	27C	280	51.260
	28CB	27C	27CG	152.23
	280	27C	27CG	126.78
	27C	270	28N	29.360
40	27C	270	27CA	32,830
	27C	270	27CB	65.400
	27C	270	28CA	60.270
	27C	270	27N	40.420
				423

	WO 03/048733			
	27C	270	72N	119.25
	27C	270	72CA	115.84
	27C	270	28C	67.810
	27C	270	72CB	133.62
5	28N	270	27CA	62.190
	28N	270	27CB	94.090
	28N	270	28CA	30.930
	28N	270	27N	65.570
	28N	270	72N	123.25
. 10	28N	270	72CA	107.43
	28N	270	28C	41.640
	28N	270	72CB	115.21
	27CA	270	27CB	33.760
	27CA	270	28CA	93.110
15	, 27CA,	270	27N	24.070
	27CA	270	72N	106.33
	27CA	270	72CA	117.49
	27CA	270	28C	98.190
	27CA	270	72CB	141.08
20	27CB	270	28CA	124.52
	27CB	270	27N	46.720
	27CB	270	72N	98.900
	· 27CB	270	72CA	120.62
	27CB	270	28C	121.57
25.	27CB	270	72CB	137.19
	28CA	270	27N	93.240
	28CA	270	72N	116.21
	28CA	270	72CA	93.160
	28CA	270	28C	23.060
30	28CA	270	72CB	91.060
	27N	270	72N	84.810
	27N	270	72CA	93.480
	27N	270	28C	106.96
	27N	270	72CB	117.07
35	72N	270	72CA	24.250
	72N	270	28C	134.35
	72N	270	72CB	39.290
	72CA	270	28C	110.11
	72CA	270	72CB	23.590
40	28C	270	72CB	100.52
	27C	28N	28CA	123.27

27C

27C

28N

28N

424

26.990

144.68

270

28CB

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	27C	28N	27CA	34.730
	27C	28N	28C	123.32
	27C	28N	280	126.47
	· 27C	28N	27N	49.740
5	27C	28N	28CG	128.18
	27C	28N	29N	114.65
	27C	28N	27CB	22.340
	28CA	. 28N	270	96.310
	28CA	28N	28CB	37.450
10	28CA	28N	27CA	157.96
	28CA	28N	28C	35.130
	28CA	28N	280	59.120
	28CA	28N	27N	150.28
	28CA	28N	28CG	32.800
15	28CA	28N	29N	28.800
	28CA	28N .	27CB	143.49
	270	28N	28CB	123.25
	270	28N	27CA	61.720
	270	28N	28C	101.36
20	270	28N	280	114.28
	270	28N	27N	73.310
	270	28N	28CG	106.86
	270	28N	29N	90.580
	270	28N	27CB	48.200
25	28CB	28N	27CA	153.91
	28CB	28N	28C	61.510
	28CB	28N	280	74.560
	28CB	28N	27N	126.83
••	28CB	28N	28CG	16.730
30	28CB	28N	29N	62.020
	28CB	28N	27CB	163.11
	27CA	28N	28C	144.55
	27CA	28N	280	129.18
25	27CA	28N	27N	27.080
35	27CA	28N	28CG	147.04
	27CA	28N	29N	142.51
	27CA	28N	27CB	16.430
*	28C	28N	280	25.920
40	28C	28N	27N	171.56
40	28C	28N	28CG	64.910
	28C	28N	29N	12.790
	28C	28N	27CB	130.53
	280	28N	27N	150.57
				425

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	•	280		28N	28CG	83.730	
		280		28N	, 29N	37.940	•
		280		28N	27CB	121.55	
		27N	• •	28N	28CG	122.57	
5		27N	•	28N	29N	163.88	
		27N		28N	. 27CB	41.090	
		28CG		28N	29N	61.280	
		28CG	٠.	28N	27CB	148.65	
		29N		28N	27CB	126.52	
10		28N		28CA	28CB	107.02	
		28N		28CA	28C	112.05	
		28N		28CA	280	89.640	•
		28N		28CA	27C	26.940	
		28N		28CA	29N	134.67	,
15		28N		28CA	28CG	128.94	$\mathbf{r} = \mathbf{r}_{\mathbf{q}} + \mathbf{r}_{\mathbf{q}} = \mathbf{r}_{\mathbf{q}}$
		28N		28CA	270	52.760	•
		28N		28CA	280D1	152.34	
		28N		28CA	280D2	113.57	1 1
		28N		28CA	. 27CA	13.760	•
20		28N		28CA	29CA	127.71	
	•	28N		28CA	72CD1	129.63	,
		28CB		28CA	28C	109.05	
	,	,28CB		28CA.	280	105.11	daren a gregoria
		28CB		28CA	27C	125.81	,
25		28CB		28CA	29N	108.67	And the second second
		28CB		28CA	28CG	32.900	
		28CB		28CA	270	139.28	
		28CB	·.	28CA	280D1	49.370	•
		28CB		28CA	280D2	36.310	
30		28CB	•	28CA	27CA	116.48	
		28CB		28CA	29CA	108.66	•
		28CB		28CA	72CD1	91.900	**
		28C		28CA	280	26.130	
		28C		28CA	27C	114.99	
35		28C		28CA	29N	28.520	
		28C		28CA	28CG	111.90	
		28C		28CA	270	111.43	
		28C		28CA	28OD1	91.730	
		28C		28CA	280D2	129.48	
40		28C		28CA	27CA	114.99	
		28C		28CA	29CA	18.660	
		28C		28CA	72CD1	104.41	
		280		28CA	27C	101.07	
						426	

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	WO 03/048733			
	280	28CA	29N	54.660
	280	28CA	28CG	122.89
	280	28CA	270	109.10
	280	28CA	280D1	109.04
5	280	28CA	280D2	138.00
	280	28CA	27CA	96.260
	280	28CA	29CA	44.780
	280	28CA	72CD1	130.51
	27C	28CA	29N	125.15
10	27C	28CA	28CG	133.04
•	27C	28CA	270	25.830
	27C	28CA	280D1	149.66
	27C	28CA	280D2	115.49
	27C	28CA	27CA	13.230
15	27C	28CA	29CA	123.17
	27C	28CA	72CD1	105.64
	29N	28CA	28CG	95.780
	29N	28CA	270	108.87
	29N	28CA	280D1	72.600
20	29N	28CA	280D2	111.76
	29N	28CA	27CA	131.70
	29N	28CA	29CA	9.900
	29N	28CA	72CD1	75.920
0.5	28CG	28CA	270	127.43
25	28CG	28CA	280D1	23.400
	28CG	28CA	280D2	17.580
	28CG	28CA	27CA	131.69
	28CG	28CA	29CA	101.05
30	28CG	28CA	72CD1	59.120
50	270	28CA	280D1	132.28
	270	28CA	280D2	112.81
	270	28CA	27CA	39.060
	270	28CA	29CA	111.06
35	270 280D1	28CA	72CD1	82.410
33		28CA	280D2	39.380
	280D1	28CA	27CA	153.28
	280D1	28CA	29CA	78.560
	280D1 280D2	28CA 28CA	72CD1	50.890
40	280D2	28CA 28CA	27CA	114.54
10	280D2	28CA 28CA	29CA	117.93
	27CA	28CA	72CD1	59.590
	27CA	28CA	29CA	127.25
	2708	ZUCA	72CD1	117.24

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	29CA	28CA	72CD1	85.820
	28CG	28CB	28CA	113.35
	28CG	28CB	280D2	28.210
	28CG	28CB	280D1	27.410
5	28CG	28CB	28N	135.71
	28CG	28CB	28C	115.15
	28CG	28CB	280	133.29
•	28CG	28CB	29N	93.780
	28CG	28CB	27C	123.45
- 10	28CA	28CB	280D2	120.99
	28CA	28CB	280D1	101.24
	28CA	28CB	28N	35.530
	28CA	28CB	28C	35.780
	28CA	28CB	280	47.240
15	. 28CA.	28CB	29N	45.280
	28CA	28CB	27C	33.900
	280D2	28CB	280D1	55.620
	280D2	28CB	28N	124.28
	280D2	28CB	28C	138.72
20	280D2	28CB	280	159.46
	280D2	28CB	29N	118.99
	280D2	28CB	27C	112.73
	280D1	28CB	28N	134.80
	280D1	28CB	28C	90.710
25	280D1	28CB	280	106.63
	280D1	28CB	29N	69.220
	280D1	28CB	27C	126.18
	28N	28CB	28C	61.110
	28N	28CB	280	58.660
30	28N	28CB	29N	77.910
	28N	28CB	27C	12.440
	28C	28CB	280	21.080
	28C	28CB	29N	21.570
	28C	28CB	27C	65.640
35	280	28CB	29N	40.530
	280	28CB	27C	67.460
	29N	28CB	27C	79.030
	280D1	28CG	280D2	123.68
	280D1	28CG	28CB	119.02
40	280D1	28CG	28CA	102.89
	280D1	28CG	72CD1	65.440
	280D1	28CG	28C	81.670
	280D1	28CG	72CE1	45.630
				420

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	280D1	28CG	28N	121.14
	280D1	28CG	29N	61.710
	28OD2	28CG	- 28CB	117.30
	280D2	28CG	28CA	124.73
5	280D2	2,8CG	72CD1	92.190
	280D2	28CG	28C	149.60
	280D2	28CG	72CE1	94.670
	28OD2	28CG	28N	108.81
•	280D2	28CG	. 29N	157.61
10	28CB	28CG	28CA	33.750
	28CB	28CG	72CD1	114.38
	28CB	28CG	28C	41.560
	28CB	28CG	72CE1	131.88
	28CB	28CG	28N	27.570
15	28CB	28CG	29N	62.520
	28CA	28CG	72CD1	80.800
	28CA	· 28CG	28C	24.870
	28CA	28CG	72CE1	98.780
	28CA	28CG	28N	18.260
20	28CA	28CG	29N	41.560
	72CD1	28CG	28C	83.390
	72CD1	28CG	72CE1	23.830
	72CD1	28CG	28N	89.660
	72CD1	28CG	29N	69.760
25	28C	28CG	72CE1	93.160
	28C	28CG	28N	41.390
	28C	28CG	29N	21.080
	72CE1	28CG	28N	111.07
	72CE1	28CG	29N	74.320
30	28N	28CG	29N	59.690
	28CG	280D1	280D2	28.200
	28CG	280D1	28CB	33.570
	28CG	280D1	72CE1	115.15
o =	28CG	280D1	28CA	53.710
35	, 28CG	280D1	72CD1	92.900
	28CG	280D1	29N	98.940
	28CG	280D1	28C	77.530
	28CG	280D1	72CZ	114.77
40	280D2	280D1	28CB	61.770
40	280D2	280D1	72CE1	98.870
	280D2	280D1	28CA	78.700
	280D2	280D1	72CD1	85.680

280D2

280D1

123.95

29N

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	280D2	280D1	28C	104.36
	280D2	280D1	, 72CZ	92.370
	28CB	280D1	72CE1	128.09
	28CB	280D1	28CA	29.390
5	28CB	280D1	72CD1	100.88
	28CB	280D1	29N	68.830
	28CB	280D1	28C	46.320
	28CB	280D1	72CZ	137.45
	72CE1	280D1	28CA	104.36
10	72CE1	280D1	72CD1	27.220
	72CE1	280D1	29N	91.190
	72CE1	280D1	28C	106.70
	72CE1	280D1	72CZ	17.090
	28CA	280D1	72CD1	78.500
15	28CA	280D1	29N	45.550
	28CA	280D1	28C	26.560
	28CA	280D1	72CZ	118.77
	72CD1	280D1	29N	78.970
	72CD1	280D1	28C	87.210
20	72CD1	280D1	72CZ	40.290
	29N	280D1	28C	22.570
	29N	280D1	72CZ	107.81
	28C	280D1	72CZ	123.75
	28CG	280D2	280D1	28.120
25	28CG	280D2	· 28CB	34.490
	28CG	280D2	28CA	37.690
	28CG	280D2	72CD1	67.750
	28CG	280D2	72CE1	65.900
	280D1	280D2	28CB	62.620
30	280D1	280D2	28CA	61.920
	280D1	280D2	72CD1	57.260
	280D1	280D2	72CE1	45.610
	28CB	280D2	28CA	22.700
	28CB	280D2	72CD1	86.670
35	28CB	280D2	72CE1	94.290
	28CA	28OD2	72CD1	66.750
	28CA	28OD2	72CE1	79.190
	72CD1	280D2	72CE1	21.880
	280	28C	29N	122.03
40	280	28C	28CA	120.19
	280	28C	29CA	90.290
	280	28C	28N	91.640
	280	28C	28CB	111.86
		•		420

	WO 03/048733			
	280	28C	27C	96.690
	280	28C	28CG	131.90
	280	28C	280D1	139.06
	280	28C	29C	89.870
5	280	28C	270	110.57
	280	28C	30N	98.730
	29N	28C	28CA	117.78
	29N	28C	29CA	31.750
	29N	28C	28N	142.75
10	29N	28C	28CB	114.75
	29N	28C	27C	128.76
	29N	28C	28CG	91.670
	29N	28C	280D1	71.910
	29N	28C	29C	37.100
15	29N	28C	270	109.27
	29N	28C	30N	42.660
	28CA	28C	29CA	149.50
	28CA	28C	28N	32.820
	28CA	28C	28CB	35.180
20	28CA	28C	27C	40.710
	28CA	28C	28CG	43.230
	28CA	28C	280D1	61.710
	28CA	28C	29C	144.76
	28CA	28C	270	45.510
25	28CA	28C	30N	126.41
	29CA	28C	28N	164.06
	29CA	28C	28CB	135.61
	29CA	28C	27C	145.15
	29CA	28C	28CG	116.00
30	29CA	28C	280D1	95.230
	29CA	28C	29C	20.590
	29CA	28C	270	128.30
	29CA	28C	30N	40.330
	28N	28C	28CB	57.390
35	28N	28C	27C	19.020
	28N	- 28C	28CG	73.700
	28N	28C	280D1	93.660
	28N	28C	29C	143.57
	28N	28C	270	37.000
40	28N	28C	30N	123.80
	28CB	28C	27C	72.390
	28CB	28C	28CG	23.290
	28CB	28C	280D1	42.970

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	28CB	28C	29C	151.53
	28CB	28C	270	80.610
•	28CB	28C	30N	149.41
	27C	28C	28CG	83.910
5	27C	28C	280D1	101.30
	27C	28C	29C	124.95
	27C	28C	270	19.530
	27C	28C	30N	104.83
	28CG	28C	280D1	20.800
10	28CG	28C	29C	128.73
	28CG	28C	270	84.850
	28CG	28C	30N	127,.77
•	280D1	28C	29C	108.58
	280D1	28C	270	97.440
15	280D1	28C	30N	111.48
	29C	28C	270	109.67
	29C	28C	30N	20.910
	270	28C	30N	88.790
	28C	280	29N	30.260
20	28C	280	28CA	33.680
	28C	280	29CA	62.770
	28C	280	28N	62.440
	28C	280	28CB	47.070
	28C	280	29C	70.870
25	. 28C	280	27C	64.340
	29N	280	28CA	63.940
	29N	280	29CA	32.520
	29N	280	28N	91.600
20	29N	280	28CB	72.570
30	29N	280	29C	42.980
	29N	280	27C	89.830
	28CA	280	29CA	96.440
	28CA	280	28N	31.240
25	28CA	280	28CB	27.650
35	28CA	280	29C	102.81
	28CA	280	27C	39.860
	29CA	280	28N	123.14
	29CA	280	28CB	101.00
40	29CA	280	29C	20.550
40	29CA	280	27C	117.68
	28N	280	28CB	46.780
	28N	280	29C	121.50
	28N	280	27C	16.540

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	28CB	280	29C	115.55
	28CB	280	27C	61.280
	29C	280	27C	110.43
•	28C	29N	29CA	119.54
5	28C	29N	280	27.710
	28C	29N	28CA	33.700
	28C	29N	29C	124.80
	28C	29N	30N	119.21
	28C	29N	28CB	43.680
10	28C	29N	280D1	85.520
, 10	28C	29N	200D1 28N	24.470
	28C	29N 29N	290	124.97
	28C	29N	28CG	67.240
	29CA	29N	280	91.840
15	29CA	29N	28CA	153.19
	29CA	29N	29C	30.470
٠	29CA	29N	30N	57.840
	29CA	29N	28CB	143.85
	29CA	29N	280D1	130.87
20	29CA	29N	28N	140.42
	29CA	29N	290	20.390
	29CA	29N	28CG	145.23
	280	29N	28CA	61.410
•	280	29N	29C	100.82
25	280	29N	30N	105.29
	280	29N	28CB	66.900
	280	29N	280D1	105.70
	280	29N	28N	50.460
	280	29N	290	98.780
30	280	29N	28CG	90.190
	28CA	29N	29C	148.72
	28CA	29N	30N	127.48
	28CA	29N	28CB	26.040
	28CA	29N	280D1	61.840
35	28CA	29N	28N	16.530
	28CA	29N	290	154.26
	28CA	29N	28CG	42.650
•	29C	29N	30N	27.380
•	29C	29N	28CB	167.69
40	29C	29N	280D1	148.53
	29C	29N	28N	132.65
	29C	29N	290	10.120
	29C	29N	28CG	167.76
				133

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	30N	29N	28CB	153.45
	30N	29N	280D1	147.27
	30N	29N	. 28N	114.75
	30N	29N	290	37.500
5	30N	29N	28CG	153.02
	28CB	29N	280D1	41.940
	28CB	29N	28N	40.060
	.28CB	29N	290	162.27
	28CB	29N	28CG	23.710
10	280D1	29N	28N	78.310
	280D1	29N	290	143.62
	280D1	29N	28CG	19.360
	28N	29N	290	137.73
	28N	29N	28CG	59.030
15	290	29N	28CG	162.19
	29N	29CA	29C	120.43
	29N	29CA	290	147.28
	29N	29CA	28C	28.710
	29N	29CA	30N	91.970
20	29N	29CA	280	55.640
	29N	29CA	30CA	102.08
	29N	29CA	28CA	16.910
•	29C	29CA	290	26.900
	29C	29CA	28C	125.53
25 [.]	29C	29CA	30N	28.490
	29C	29CA	280	120.71
	29C	29CA	30CA	18.360
	29C	29CA	28CA	125.32
	290	29CA	28C	146.41
30	290	29CA	30N	55.390
	290	29CA	280	129.18
	290	29CA	30CA	45.260
	290	29CA	28CA	150.37
	· 28C	29CA	30N	100.21
35	28C	29CA	280	26.940
	28C	29CA	30CA	109.44
	28C	29CA	28CA	11.840
	30N	29CA	280	105.06
	30N	29CA	30CA	10.130
40	30N	29CA	28CA	97.730
	280	29CA	30CA	111.26
	280	29CA	28CA	38.780
	30CA	29CA	28CA	107.63
				434

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	290	· 29C	30N	122.23
	290	29C	29CA	119.22
	290	29C	30CA	90.610
	290	' 29C	29N	148.27
5	290	29C	30C	72.390
	290	29C	31N	81.660
	290	29C	28C	145.21
	290	29C	30CB	106.09
	290	29C	280	128.94
10	290	29C	30ND2	114.58
	290	, 29C	300	59.110
	30N	29C	29CA	118.55
	30N	29C	30CA	31.620
	30N	29C	29N	89.480
15	30N	29C	30¢	55.670
	30N	29C	31N	62.350
	30N	29C	28C	88.620
	30N	29C	30CB	16.150
	30N	29C	280	96.860
20	30N	29C	30ND2	34.300
	30N	29C	300	65.850
	29CA	29C	30CA	150.17
	29CA	29C	29N	29.100
	29CA	29C	30C	154.01
25	29CA	29C	31N	129.42
	29CA	29C	28C	33.880
	29CA	29C	30CB	134.69
	29CA	29C	280	38.750
	29CA	29C	30ND2	114.59
30	29CA	29C	300	163.18
	30CA	29C	29N	121.08
	30CA	29C	30C	30.880
	30CA	29C	31N	49.750
	30CA	29C	28C	118.92
35	30CA	29C	30CB	15.480
	30CA	29C	280	122.44
	30CA	29C	30ND2	44.530
	30CA	29C	300	36.420
	29N	29C	30C	134.46
40	29N	29C	31N	116.51
	29N	29C	28C	18.100
	29N	29C	30CB	105.61
	29N	29C	280	36.200
				435

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		1.		
•	29N	29C	30ND2	91.810
	29N	29C	, 300	148.84
	30C	29C	31N	24.920
	30C	29C	28C	142.20
5	30C	29C	30CB	41.950
	30C	29C	280	152.26
	30C	29C	30ND2	75.400
	30C	. 29C	300	14.380
	31N	29C	28C	130.82
10	31N	. 29C	30CB	54.430
	31N	29C	280	149.26
	31N	29C	30ND2	91.600
	31N	29C	300	35.810
	28C	29C	30CB	104.20
15	28C	29C	280	19.260
	28C	29C	30ND2	80.950
	28C	29C	300	154.43
	30CB	29C	280	110.33
	30CB	29C	30ND2	37.220
20	30CB	29C .	300	50.510
	280	29C	30ND2	78.810
	280	29C	300	156.96
	30ND2	29C	, , , 300, ,	78,.52 <u>0</u>
	29C	290	30N	30.100
25	29C	290	29CA	33.880
	29C	290	30CA	62.390
	29C	290	30C	83.190
	29C	290	31N	76.100
	29C	290	300	102.69
30	29C	290	32N	109.56
	29C	290	29N	21.600
	29C	290	32C	146.61
	30N	290	29CA	63.980
	30N	290	30CA	32.290
35	30N	290	30C	56.600
	30N	290	31N	58.480
	30N	290	300	74.320
	30N	290	32N	106.90
	30N	290	29N	51.700
40	30N	290	32C	139.48,
	29CA	290	30CA	96.270
	29CA	290	30C	113.67
	29CA	290	31N	98.860
				436

29CA 290 300 134 0 29CA 290 32N 106 3 29CA 290 29N 12 3 29CA 290 32C 130 6 5 30CA 290 30C 31 7 30CA 290 30N 44 6 30CA 290 32N 98 8 30C 290 31N 24 6 30C 290 31N 24 6 30C 290 300 20 6 30C 290 30N 30 88 6 31N 290 32N 68 6 31N 290 32N 51 8 31N 290 32N 67 6 31N 290 32C 37 8 32N 290 32N 107 3 32N 290 32N 107 3 32N 290 32N 107 3 32N 290 32N 30CA 119 6 29C 30N 30CB 155 1 29C 30N 30CB 155 1 29C 30N 30ND2 129 9	3 20 2 60 90 20 40 70
29CA 290 29N 12.3 29CA 290 32C 130.8 29CA 290 30C 31.3 30CA 290 31N 47.8 30CA 290 300 44.4 30CA 290 32N 98.5 30CA 290 32N 98.5 30CA 290 32N 98.5 30CA 290 32N 98.5 30C 290 31N 24.4 30C 290 300 20.4 30C 290 30N 20C 116.6 30C 290 32N 68.4 30C 290 32N 68.6 30C 290 32N 68.6 30C 290 32N 68.6 30C 290 32N 68.6 31N 290 32C 85.9 31N 290 32C 85.9 31N 290 32N 51.9 31N 290 32N 67.4 30C 290 32N 67.4 31N 290 32C 81.0 31N 290 32C 81.0 31N 290 32C 81.0 31N 290 32C 81.0 32N 290 32C 72.8 32N 290 32C 37.5 29C 30N 30CA 119.6 29C 30N 30CB 155.1 29C 30N 30CB 155.1 29C 30N 30ND2 129.9 30C 29C 30N 30ND2 129.9 30C 29C 30N 30ND2 129.9	20 20 90 20 40 70
29CA 290 32C 130.8 30CA 290 30C 31.7 30CA 290 31N 47.8 30CA 290 300 44.4 30CA 290 32N 98.5 30CA 290 32C 116.6 30C 290 31N 24.4 30C 290 300 20.4 30C 290 32N 68.4 31N 290 32N 51.9 31N 290 32N 51.9 31N 290 32N 51.9 31N 290 32N 67.4 30O 290 32N 67.4 30O 290 32C 72.8 32N 290 32C 72.8	2 60 90 20 40 70
5 30CA 290 30C 31.7 47.5 30CA 290 31N 47.5 30CA 290 300 44.4 30CA 290 32N 98.5 30CA 290 32N 98.5 30CA 290 32C 116.6 30CA 290 32C 116.6 30CA 290 32N 68.4 30CA 32N 32CA	60 90 20 40 70
30CA 290 31N 47.5 30CA 290 300 44.4 30CA 290 32N 98.5 30CA 290 29N 83.9 30CA 290 32C 116.6 30C 290 31N 24.4 30C 290 300 20.4 30C 290 32N 68.4 30C 290 32N 68.6 31N 290 32C 85.9 31N 290 32C 85.9 31N 290 32C 85.9 31N 290 32N 51.9 31N 290 32N 51.9 31N 290 32N 51.9 31N 290 32C 81.0 31N 290 32C 81.0 32N 290 32C 72.8 32N 290 32C 72.8 32N 290 32C 72.8 32N 290 32C 37.5 29C 30N 30CA 119.6 29C 30N 30CB 155.1 29C 30N 30CB 155.1 29C 30N 30CB 155.1	90 20 40 70
30CA 290 300 44.4 30CA 290 32N 98.5 30CA 290 29N 83.9 30CA 290 32C 116.6 30C 290 31N 24.4 30C 290 300 20.4 30C 290 300 20.4 30C 290 32N 68.4 30C 290 32N 68.4 30C 290 32N 68.4 30C 290 32N 68.4 31N 290 32N 51.5 31N 290 32C 85.5 31N 290 32N 67.4 300 290 32N 67.4 300 290 32N 67.4 300 290 32N 67.4 300 30N 30CA 119.6 30C 29C 30N 30CB 155.1 30C 29C 30N 30ND2 129.5 30O 29C 30N 30ND2 129.5	20 40 70 7
30CA 290 32N 98.5 30CA 290 29N 83.9 10 30CA 290 32C 116.6 30C 290 31N 24.4 30C 290 300 20.4 30C 290 32N 68.4 30C 290 32N 68.4 30C 290 32N 68.4 30C 290 32N 68.4 31N 290 32C 85.9 31N 290 32N 51.9 31N 290 32N 51.9 31N 290 32N 51.9 31N 290 32C 81.0 31N 290 32C 81.0 31N 290 32C 81.0 31N 290 32C 81.0 32N 290 32C 72.6 32N 290 32C 72.6 32N 290 32C 37.5 32N 290 32C 37.5 32N 290 32C 37.5 32N 290 32C 37.5 32N 290 32C 37.6 32N 29C 30N 30CA 119.6 29C 30N 30CB 155.1 29C 30N 30CB 155.1 29C 30N 30CB 155.1 29C 30N 30ND2 129.9 29C 30N 30ND2 129.9	40 70 7
30CA 290 29N 83.5 10 30CA 290 32C 116.6 30C 290 31N 24.4 30C 290 300 20.4 30C 290 32N 68.4 30C 290 32N 68.4 30C 290 32N 68.5 31N 290 32C 85.5 31N 290 300 39.7 31N 290 32N 51.5 31N 290 32N 51.5 31N 290 32N 51.5 31N 290 32C 81.0 20 300 290 32N 67.4 300 290 32N 67.4 300 290 32C 72.6 32N 290 32C 72.6 32N 290 32C 37.5 25 29N 290 32C 37.5 29C 30N 30CA 119.6 29C 30N 30CB 155.1 29C 30N 30CB 155.1 29C 30N 30CB 77.8 30 29C 30N 30CD 129.9 30 29C 30N 30ND2 129.9 30 29C 30N 30ND2 129.9	70 7
10 30CA 290 32C 116.6 30C 290 31N 24.6 30C 290 300 20.6 30C 290 32N 68.6 30C 290 32N 68.6 30C 290 32N 68.6 31N 290 32C 85.9 31N 290 300 39.7 31N 290 32N 51.9 31N 290 32N 51.9 31N 290 32C 81.0 32N 290 32C 72.6 32N 290 32C 72.6 32N 290 32C 72.6 32N 290 32C 37.5 29C 30N 30CA 119.6 29C 30N 30CB 155.1 29C 30N 30CB 155.1 29C 30N 30CB 155.1 29C 30N 30CB 77.8 30 29C 30N 30CB 155.1	7
30C 290 31N 24.4 30C 290 300 20.4 30C 290 32N 68.4 30C 290 29N 102.3 31N 290 32C 85.9 31N 290 300 39.7 31N 290 32N 51.9 31N 290 32N 51.9 31N 290 32C 81.0 31N 290 32C 81.0 31N 290 32C 81.0 31N 290 32C 81.0 32N 290 32N 67.4 300 290 32N 67.4 300 290 32C 72.8 32N 290 32C 72.8 32N 290 32C 37.5 32N 290 32C 37.5 29C 30N 30CA 119.6 29C 30N 30CB 155.1 29C 30N 30CB 155.1 29C 30N 30CB 155.1 29C 30N 30CB 77.8 32N 29C 30N 30CB 155.1	
30C 290 300 20.4 30C 290 32N 68.4 30C 290 29N 102.3 30C 290 32C 85.9 31N 290 300 39.7 31N 290 32N 51.9 31N 290 32N 51.9 31N 290 32C 81.0 31N 290 32C 81.0 31N 290 32C 81.0 31N 290 32C 81.0 300 290 32N 67.4 300 290 32C 72.8 32N 290 32C 72.8 32N 290 32C 72.8 32N 290 32C 37.5 32N 290 32C 37.5 29C 30N 30CA 119.6 29C 30N 30CB 155.1 29C 30N 30CB 155.1 29C 30N 30CB 155.1 29C 30N 30CB 77.8 32N 29C 30N 30CB 155.1	20
30C 290 32N 68.4 30C 290 29N 102.3 31N 290 32C 85.9 31N 290 32N 51.9 31N 290 32N 51.9 31N 290 32N 51.9 31N 290 32C 81.0 31N 290 32C 81.0 31N 290 32C 81.0 300 290 32N 67.4 300 290 32N 67.4 300 290 32C 72.8 32N 290 32C 72.8 32N 290 32C 37.5 32N 290 32C 37.5 29C 30N 30CA 119.6 29C 30N 30CB 155.1 29C 30N 30CB 155.1 29C 30N 30CB 155.1 29C 30N 30CB 77.8 29C 30N 30CB 155.1	
30C 290 29N 102.3 30C 290 32C 85.3 31N 290 300 39.7 31N 290 32N 51.3 31N 290 29N 89.3 31N 290 32C 81.0 31N 290 32C 81.0 31N 290 32C 81.0 300 290 32N 67.4 300 290 32N 67.4 300 290 32C 72.8 32N 290 32C 72.8 32N 290 32C 37.5 29C 30N 30CA 119.6 29C 30N 30CB 155.1 29C 30N 30CB 155.1 29C 30N 30CB 155.1 29C 30N 30CB 77.8 29C 30N 30CB 77.8 29C 30N 30CB 155.1 29C 30N 30CB 77.8 29C 30N 30CB 155.1 29C 30N 30CB 77.8 29C 30N 30CB 77.8 29C 30N 30CB 129.9 30C 30N 30CD 129.9	10
15 30C 290 32C 85.9 31N 290 300 39.7 31N 290 32N 51.9 31N 290 29N 89.9 31N 290 32C 81.0 31N 290 32C 81.0 300 290 32N 67.4 300 290 32N 67.4 300 290 32C 72.8 32N 290 32C 72.8 32N 290 32C 37.5 32N 290 32C 37.5 29C 30N 30CA 119.6 29C 30N 30CB 155.1 29C 30N 30CB 155.1 29C 30N 30CB 32.9 30 29C 30N 30ND2 129.9 29C 30N 30ND2 129.9	50
31N 290 300 39.7 31N 290 32N 51.9 31N 290 29N 89.9 31N 290 32C 81.0 31N 290 32C 81.0 300 290 32N 67.4 300 290 32N 67.4 300 290 32C 72.8 32N 290 32C 72.8 32N 290 32C 37.5 29C 30N 30CA 119.6 29C 30N 30CB 155.1 29C 30N 30CB 155.1 29C 30N 30CB 32.9 30 29C 30N 30CD 97.8 29C 30N 30ND2 129.9 29C 30N 30ND2 129.9	0
31N 290 32N 51.9 31N 290 29N 89.9 31N 290 32C 81.0 31N 290 32C 81.0 31N 290 32C 81.0 300 290 32N 67.4 300 290 32C 72.8 32N 290 32C 72.8 32N 290 32C 37.5 32N 290 32C 37.5 29C 30N 30CA 119.6 29C 30N 29CA 32.9 300 29C 30N 30CD 129.9 29C 30N 30ND2 129.9 29C 30N 30ND2 129.9	80
31N 290 29N 89.5 31N 290 32C 81.0 31N 290 32C 81.0 300 290 32N 67.4 300 290 32C 72.8 32N 290 32C 72.8 32N 290 32C 37.5 32N 290 32C 37.5 29C 30N 30CA 119.6 29C 30N 30CB 155.1 29C 30N 30CB 155.1 29C 30N 30C 97.8 29C 30N 30CD 97.8 29C 30N 30ND2 129.9 29C 30N 30ND2 129.9	70
31N 290 32C 81.0 20 300 290 32N 67.4 300 290 29N 122.5 300 290 32C 72.8 32N 290 29N 107.3 32N 290 32C 37.5 29C 30N 30CA 119.6 29C 30N 30CA 119.6 29C 30N 30CB 155.1 29C 30N 30CB 155.1 29C 30N 29CA 32.9 30 29C 30N 30ND2 129.9 29C 30N 31N 92.7	90
20 300 290 32N 67.4 300 290 29N 122.5 300 290 32C 72.6 32N 290 29N 107.3 32N 290 32C 37.5 25 29N 290 32C 137.6 29C 30N 30CA 119.6 29C 30N 29O 27.6 29C 30N 30CB 155.1 29C 30N 30CB 155.1 29C 30N 30CD 97.8 29C 30N 30ND2 129.9 29C 30N 30ND2 129.9 29C 30N 30ND2 129.9 29C 30N 31N 92.7	20
300 290 29N 122.5 300 290 32C 72.6 32N 290 29N 107.3 32N 290 32C 37.5 29C 30N 30CA 119.6 29C 30N 29O 27.6 29C 30N 30CB 155.1 29C 30N 29CA 32.9 30 29C 30N 30CD 97.8 29C 30N 30CD 129.9 29C 30N 30ND2 129.9	50
300 290 32C 72.8 32N 290 29N 107.3 32N 290 32C 37.5 32N 290 32C 37.5 29C 30N 30CA 119.6 29C 30N 290 27.6 29C 30N 30CB 155.1 29C 30N 29CA 32.9 30 29C 30N 30CD 97.8 29C 30N 30ND2 129.9 29C 30N 30ND2 129.9	40
32N 290 29N 107.3 32N 290 32C 37.5 290 32C 137.8 290 30N 30CA 119.6 290 30N 290 27.6 290 30N 30CB 155.1 290 30N 29CA 32.9 300 29C 30N 30C 97.8 29C 30N 30ND2 129.9 29C 30N 31N 92.7	4
32N 290 32C 37.5 25 29N 290 32C 137.6 29C 30N 30CA 119.6 29C 30N 290 27.6 29C 30N 30CB 155.1 29C 30N 29CA 32.9 30 29C 30N 30C 97.8 29C 30N 30ND2 129.9 29C 30N 31N 92.7	60
25 29N 29O 32C 137.8 29C 30N 30CA 119.6 29C 30N 29O 27.6 29C 30N 30CB 155.1 29C 30N 29CA 32.9 30 29C 30N 30C 97.8 29C 30N 30ND2 129.9 29C 30N 31N 92.7	9
29C 30N 30CA 119.6 29C 30N 29O 27.6 29C 30N 30CB 155.1 29C 30N 29CA 32.9 30 29C 30N 30C 97.8 29C 30N 30ND2 129.9 29C 30N 31N 92.7	00
29C 30N 29O 27.6 29C 30N 30CB 155.1 29C 30N 29CA 32.9 30 29C 30N 30C 97.8 29C 30N 30ND2 129.9 29C 30N 31N 92.7	8
29C 30N 30CB 155.1 29C 30N 29CA 32.9 30 29C 30N 30C 97.8 29C 30N 30ND2 129.9 29C 30N 31N 92.7	1
29C 30N 29CA 32.9 30 29C 30N 30C 97.8 29C 30N 30ND2 129.9 29C 30N 31N 92.7	70
30 29C 30N 30C 97.8 29C 30N 30ND2 129.9 29C 30N 31N 92.7	3
29C 30N 30ND2 129.9 29C 30N 31N 92.7	60
29C 30N 31N 92.7	80
·	3
29C 20M 20M 62.1	60
29C 30N 29N 63.1	30
29C 30N 30CG 154.9	3
35 29C 30N 30O 93.9	70
29C 30N 28C 70.4	60
30CA 30N 29O 91.9	50
30CA 30N 30CB 35.5	20
30CA 30N 29CA 152.5	7
40 30CA 30N 30C 34.9	60
30CA 30N 30ND2 70.2	
30CA 30N 31N 60.4	10

30CA

30N

29N

176.68

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	30CA	30N	30CG	57.170
	30CA	30N	300	30.530
	30CA	30N	28C	162.37
	290	- 30N	30CB	127.47
5	290	30N	29CA	60.630
	290	30N	30C	73.990
	290	30N	30ND2	123.38
	290	30N	31N	78.450
	290	30N	29N	90.800
10	290	30N	30CG	138.42
	290	30N	300	67.810
	290	30N	28C	97.020
	30CB	30N	29CA	171.88
	30CB	30N	30C	60.600
15	30CB	30N	30ND2	53.970
	30CB	30N	31N	74.000
	30CB	30N	29N	141.69
	30CB	30N	30CG	30.100
	30CB	30N	300	62.310
20	30CB	30N	28C	133.31
	29CA	30N	30C	125.63
	29CA	30N	30ND2	123.82
	29CA	30N	. 31N	109.21
	29CA	30N	29N	30.190
25	29CA	30N	30CG	145.25
	29CA	30N	300	125.03
	29CA	30N	28C	39.460
	30C	30N	30ND2	105.12
	30C	30N	31N	28.440
30	30C	30N	29N	144.78
	30C	30N	30CG	88.830
	30C	30N	300	12.250
	30C	30N	28C	162.66
	30ND2	30N	31N	126.86
35	30ND2	30N	29N	109.72
	30ND2	30N	30CG	26.110
	30ND2	30N	300	99.330
	30ND2	30N	28C	92.200
	31N	30N	29N	118.36
40	31N	30N	30CG	103.99
	31N	30N	300	39.730
	31N	30N	28C	136.29
	29N	30N	30CG	121.32
	v.			120

	WU 03/048/33			
	29N	30N	300	150,40
	29N	30N	28C	18.130
	-30CG	30N	4 300	87.520
	30CG	· 30N	28.C	107.18
5	300	30N	28C	164.36
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	30N	30CA	30C	112.03
	30N	30CA	300	131.50
	30N	30CA	29C	28.760
10	30N	30CA	31N	88.380
	30N	30CA	30CG	93.640
	30N	30CA	30ND2	78.770
	30N	30CA	290	55.760
	30N	30CA	300D1	97.290
15	30N	30CA	29CA	17.300
	30N	30CA	31CA	96.000
	30CB	30CA	30C	109.05
	30CB	30CA	300	109.06
	30CB	30CA	29C	139.47
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	30CB	30CA	30CG	33.600
	30CB	30CA	30ND2	62.890
	30CB	30CA	290	166.48
	30CB	30CA	300D1	25.650
25	30CB	30CA	29CA	128.00
	30CB	30CA	31CA	105.80
	30C	30CA	300	26.410
	30C	30CA	29C	95.100
20	30C	30CA	31N	29.210
30	30C	30CA	30CG	142.26
	30C	30CA	30ND2	168.84
	30C	30CA	290	78.730
	30C	30CA	300D1	134.55
٥.	30C	30CA	29CA	101.94
35	30C	30CA	31CA	20.100
	300	30CA	29C	106.87
	300	30CA	31N	55.620
	300	30CA	30CG	134.40
40	300	30CA	30ND2	145.73
40	300	30CA	290	82.910
	300	30CA	300D1	129.50
	300	30CA	29CA	116.83
	300	30CA	31CA	46.510

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	200	2007	211	01 420
	29C	30CA	31N	81.430
	29C	30CA	30CG	118.36 95.920
	29C	30CA	30ND2	
5	29C	30CA	290	27.000 123.63
J	29C	30CA	300D1	
	29C	30CA	29CA	11.470
	29C	30CA	31CA	85.860
	31N	30CA	30CG	134.14
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	31N	30CA	31CA	9.120
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15	30CG	30CA	290	
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·	30CG	30CA	29CA	108.76
	30CG	30CA	31CA	138.10
••	30ND2	30CA	290	110.79
20	30ND2	30CA	300D1	37.290
	30ND2	30CA	29CA	89.220
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	290	30CA	300D1	145.98
	290	30CA	29CA	38.470
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	300D1	30CA	29CA	113.33
	300D1	30CA	31CA	130.32
	29CA	30CA	31CA	89.710
	30CG	30CB	30CA	112.22
30	30CG	30CB	300D1	26.140
	30CG	30CB	30ND2	29.720
	30CG	30CB	30N	94.860
	30CG	30CB	30C	147.37
	30CG	30CB	31N	152.68
35	30CG	30CB	300	143.17
	30CG	30CB	45CD2	90.510
	30CG	30CB	29C	99.810
	30CA	30CB	300D1	138.33
	30CA	30CB	30ND2	82.530
40	30CA	30CB	30N	33.760
	30CA	30CB	30C	35.600
	30CA	30CB	31N	48.310
	30CA	30CB	300	44.510

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	30CA	30CB	45CD2	156.51
	30CA	30CB	29C	25.040
	300D1	30CB	. 30ND2	55.860
	300D1	30CB	30N	116.48
5	300D1	30CB	30C	173.05
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	300D1	30CB	300	157.21
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•	300D1	30CB	29C	123.04
10	30ND2	30CB	30N	69.900
	30ND2	30CB	30C	117.72
	30ND2	- 30CB	31N	126.99
	30ND2	30CB	300	117.84
	30ND2	30CB	45CD2	120.16
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	30N	30CB	30°C	60.230
	30N	- 30CB	31N	58.220
	30N	30CB	300	75.530
	30N	30CB	45CD2	143.63
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	30C	30CB	31N	23.510
	30C	30CB	300	19.910
	30C	30CB	45CD2	122.11
	30C	30CB	29C	53.020
25	31N	30CB	300	41.290
	31N	30CB	45CD2	108.35
	31N	30CB	29C	54.210
	300	30CB	45CD2	118.45
	300	30CB	29C	67.300
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	300D1	30CG	30CB	121.44
	300D1	30CG	30CA	155.54
	300D1	30CG	.30N	152.61
35	300D1	, 30CG	30C	141.79
	300D1	30CG	45CD2	54.230
	30ND2	30CG	30CB	115.85
	30ND2	30CG	30CA	81.700
	30ND2	30CG	30N	68.090
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	30ND2	30CG	45CD2	175.41
	30CB	30CG	30CA	34.170
	30CB	30CG	30N	55.040

	30CB	30CG	30C	20.460
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	30CA	30CG	30N	29.190
	30CA	30CG	30C	14.140
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	30N	30CG	. 30C	40.220
	30N	30CG	45CD2	112.99
	30C	· 30CG	45CD2	87.760
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	30CG	300D1	30CA	16.460
	30CG	300D1	45CA	107.38
	30ND2	300D1	30CB	62.080
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	30ND2	. 300D1	30CA	46.090
	30ND2	.300D1	45CA	123.53
	30CB	300D1	45CD2	76.330
	30CB	300D1	30CA	16.030
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	. 30CA	. 300D1	45CA	97.680
	30CG	30ND2	300D1	27.630
25	30CG	30ND2	30CB	34.430
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	30CG	30ND2	30N	85.800
	30CG	30ND2	29C	101.18
	300D1	30ND2	30CB	62.060
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	30CB	30ND2	30CA	34.590
	30CB	30ND2	30и	56.130
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	30CA	30ND2	30N	31.020
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	30N	30ND2	29C	15.760
	300	30C	31N	123.08
40	300	30C	30CA	120.03
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	300	30C	30CB	116.68
				4.40

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	300	30C	290	105.73	
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	31N	30C	32N	51.260	
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	31N	30C	310	64.140	•
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	30CA	30C	30N	33.020	
	30CA	30C	30CB	35.360	
20	30CA	30C	290	69.500	
	30CA	30C	29C	54.020	
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	30CA	30C	32N	129.67	

30CG

30ÇG

30CB

310

25 30CA 310 161.89 30C 31CA 30C 30N 118.61 31CA 30C 30CB 130.91 31CA 30C 290 104.32 31CA 30C 29C 107.30 30 28.450 31CA 30C 31C 32N 42.540 31CA 30C

30C

30CA

31CA

31CA

30N

35 30N 30C 290 49.410 30N 30C 29C 26.450 31C 118.85 30N 30C 98.490 30N 30C 32N

30C

30C

30C

30N 30C 30CG 50.950 40 133.57 30N 30C 310 104.22 30CB 30C 290 29C 85.030 30CB 30C 31C 158.64 30CB 30C

23.600

140.74

36.590

59.170

	WO 03/048733			
	30CB	30C	32N	152.48
	30CB	30C	30CG	12.170
	30CB	30C	310	162.52
	290	30C	29C	24.420
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	290	30C	32N	63.960
	290	30C	30CG	93.020
	290	. 30C	310	92.450
	29C	30C	31C	97.110
10	29C	30C	32N	75.660
	29 <u>C</u>	30C	30CG	75.610
	29C	30C	310	109.46
	31C	30C	32N	21.500
	31C	30C	30CG	164.83
15	31C	30C	310	16.550
	32N	30C	30CG	148.93
	32N	30C	310	35.130
	30CG	30C	310	174.51
	30C	300	31N	29,760
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	30C	300	31CA	61.240
	30C	300	31C	78.850
	. 30C	300	30CB	43.410
	30C	300	290	53.850
25.	30C	300	310	99.410
	30C	300	30N	25.240
	30C	300	32N	70.370
	30C	300	29C	36.790
20	31N	300	30CA	63.320
30	31N	300	31CA	31.480
	31N	300	31C	52.400
	31N	300	30CB	68.120
	31N	300	290	66.140
25	31N	300	310	71.660
35	31N	300	30N	52.660
	31N	300	32N	50.450
	31N	300	29C	55.140
	30CA	300	31CA	94.800
40	30CA	300	31C	109.50
40	30CA	300	30CB	26.430
	30CA	300	290	52.670
	30CA	300	310	130.30
	30CA	300	30N	17.970

	WO 03/048733			
	30CA	. 300	32N	96.210
	30CA	300	29C	36.710
	31CA	300	4 31C	29.120
	31CA	300	30CB	96.070
5	31CA	300	290	84.670
	31CA	300	310	43.350
	31CA	300	30N	83.140
	31CA	300	32N	39.630
	31CA	. 300	. 29C	80.440
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•	31C	300	30N	92'.960
•	31C	300	32N	19.020
15	31C	300.	29C	80.980
	30CB	3,00	290	78.960
	30CB	300	310	139.22
	30CB	300	30N	42.160
	30CB	300	32N	113.76
20	30CB	300	29C	62.190
	290	300	310	91.030
	290	300	30N	37.860
	290	300	32N	57.170
	290	300	29C	18.190
25	310	300	30N	113.40
	310	300	32N	35.790
	310	300	29C	99.540
•	30N	300	32N	78.500
20	30N	300	29C	20.180
30	32N	300	29C	63.760
	30C	31N	31CA	121.54
	30C	31N	300	27.160
	30C	31N	30CA	33,900
0.5	30C	31N	31C	104.99
35	30C	31N	,30N	61.710
	30C	31N	32N	107.97
	30C	31N	29C	69.130
	30C	31N	30CB	47.750
40	30C	31N	290	61.660
40	30C	31N	310	95.590
	31CA	31N	300	94.380
	31CA	31N	30CA	155.43
	31CA	31N	31C	33.750

	WO 03/048733			
ė	31CA	31N	30N	163.31
	31CA	31N ·	32N	55.530
•	31CA	31N	29C	138.46
	31CA	31N	30CB	147.89
5	31CA	31N	290	121.80
	31CA	31N .	310	32.550
	300	31N	30CA	61.060
	300	31N	31C	81.750
	300	. 31N	30N	87.610
10	300	31N	32N	93.250
	300	31N	29C	89.050
	300	31N	30CB	70,590
	300	31N	290	74.090
	300	31N	310	70.250
15	30CA	31N	31C	132.39
	30CA	31N	30N	31.160
•	30CA	31N	32N	121.81
	30CA	31N	29C	48.820
	30CA	31N	30CB	27.660
20	30CA	31N	290	55.240
	30CA	31N	310	127.00
,	31C	31N	30N	130.99
4		31N	. 32N	26.800
	31C	31N	29C	106.84
25	31C	31N	30CB	152.25
	31C	31N	290	88.200
	31C	31N	310	14.520
	30N	31N	32N	107.85
	30и	31N	29C	24.880
30	30N	31N	30CB	47.780
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	30N	31N	310	135.94
	32N	31N	29C	82.970
	32N	31N	30CB	149.45
35	32N	' 31N	290	68.170
	32N	31N	310	40.090
	29C	31N	30CB	71.370
	29C	31N	290	22.240
	29C	31N	310	114.32
40	30CB	31N	290	82.270
	30CB	31N	310	140.26
	290	31N	310	93.370

31N

31CA

446

114.05

31C

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		,

	31N	31CA	310	128.25
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	31C	31CA	32N	29.160
	31C	31CA	30C	101.61
10	31C	31CA	300	87.840
	31C	31CA	32CA	19.930
	31C	31CA	30CA	107.84
	310	31CA	32N	55.860
	310	31CA	30C	105.79
15	310	31CA	300	83.420
	310	31CA	32CA	46.640
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20	32N	31CA	32CA	9.260
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	30C	31CA	300	26.250
	30C	31CA	32CA	96.610
'	30C	31CA	30CA	12.440
25	300	31CA	32CA	91.250
•	300	31CA	30CA	38.700
	32CA	31CA	30CA	98.990
	310	31C	32N	123.15
	310	31C	31CA	119.67
30	310	31C	32CA	92.510
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40	32N	31C	32C	55.190
	32N	31C	300	111.38
	32N	31C	30C	99.410
	32N	31C	32CB	15.030
				447

	WO 03/048733			
	32N	31C	320	65.220
	31CA	31C	32CA	147.82
	31CA	31C	31N	32.200
	31CA	31C	32C	151.85
5	31CA	31C	300	63.040
	31CA	31C	30C	49.950
	31CA	31C	32CB	132.08
	31CA	31C	320	161.58
	32CA	31C	31N	122.49
10	32CA	, 31C	32C	31.340
	32CA	31C	300	117.61
	32CA	31C	30C	117.02
	32CA	31C	32CB	15.750
	32CA	31C	320	36.890
15	31N	31C	32C	120.12
	31N	, 31C	300	45.850
	31N	31C	30C	24.470
	31N	31C	32CB	108.34
	31N	31C	320	132.40
20	32C	31C	. 300	93.190
	32C	31C	30C	102.41
	32C	31C	32CB	41.910
	. 32C	31C		14.090
	300	31C	30C	22.760
25	300	31C	32CB	114.13
	300	31C	320	98.730
	30C	31C	32CB	107.45
	30C	31C	320	112.07
	32CB	31C	320	50.690
30	31C	310	32N	29.650
	310	310	31CA	33.620
	310	310	32CA	61.210
	31C	310	32C	80.950
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35	31C	310	300	30.520
	31C	310	31N 30C	46.190
	31C	310		63.270
	32N	310	31CA	31.570
	32N	310	32CA 32C	55.260
40	32N	310	320	72.760
	32N	310	320	80.920
	32N	310	300	55.520

32N

310

448

31N

57.120

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32N	310	30C	66.230	·	

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4		31CA	310	32C	111.03	•
	•	31CA	310	320	131.02	
	5	31CA	310	300	53.230	
		31CA	310	31N	19.200	
		31CA	310	30C	37.620	·
		32CA	310	32C	31.410	
		32CA	310	320	43.840	
	10	32CA	310	300	99.290	
	,	32CA	310	31N	86.720	
		32CA	310	30C	90.250	
		32C	310	320	19.990	
		32C	310	300	87.840	
	15	32C	310	31N	95.500	•
		32C	310	30C	88.220	
		320	310	30Ó	100.93	
		320	310	31N	115.06	•
		320	310	30C	105.40	
	20	300	310	31N	38.090	•
		300	310	30C	18.410	
		31N	310	30C	20.270	
		31C	32N	32CA	121.54	
p. 4 4		31C	32N	310	27.200	, .
•	25	31C	32N	31CA	33.670	
		31C	32N	32C	98.180	
		31C	32N	32CB	156.92	•
	,	31C	32N	31N	57.520	
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		32CA	32N	310	94.370	
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		32CA	32N	300	122.95	•
		•			449	;
						•
				•		

	WO 03/048733			
	310	32N	31CA	60.870
	310	32N	32C	75.320
	310	32N	32CB	129.85
	310	32N	31N	82.780
5	310	32N	32CG	133.06
	310	32N	290	115.44
	310	32N	320	69.350
	310	32N	30C	78.640
	310	32N	300	63.290
10	31CA	32N	32C	125.80
	31CA	32N	32CB	168.95
	31CA	32N	31N	29.530
	31CA	32N	32CG	151.44
	31CA	32N	290	88.480
15	. 31CA,	32N	320	125.80
	31CA	32N	30C	42.620
	31CA	32N	300	46.720
	32C	32N	32CB	61.170
	32C	32N	31N	122.11
20	32C	32N	32CG	82.280
	32C	32N	290	82.700
	32C	32N	320	11.910
	32C	32N	30C	101.56
	32C	32N	300	86.660
25	32CB	32N	31N	140.79
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	32CB	32N	290	83.900
	32CB	32N	320	63.040
	32CB	32N	30C	131.25
30	32CB	32N	300	131.78
	31N	32N	32CG	143.06
	31N	32N	290	59.840
	31N	32N	320	129.20
	31N	32N	30C	20.780
35	31N	32N	. 300	36.300
	32CG	32N	290	101.62
	32CG	32N	320	80.410
	32CG	32N	30C	147.03
	32CG	32N	300	155.75
40	290	32N	320	94.600
	290	32N	30C	47.590
	290	32N	300	55.390
	320	32N	30C	109.54

	WO 03/048733			
	320	32N	300	92.920
	30C	32N	300	18.840
	32N	32CA	4 32C	109.35
	32N	, 32ÇA	32CB	111.02
5	32N	32CA	320	129.14
	32N	32CA	31C	27.780
	32N	32CA	32CG	106.55
	32N	32CA	310	54.050
	32N	32CA	31CA	15.570
10	32N	32CA	32CD	105.36
	32C	32CA	32CB	109.02
	32C	32CA	320	26.200
	32C	32CA	31C	92.860
	32C	32CA	32CG	136.13
15	32C	32CA.	310	77.720
	32C	32CA	31CA	99.800
	32C	32CA	32CD	127.84
	32CB	32CA	320	109.26
	32CB	32CA	31C	138.74
20	32CB	32CA	32CG	32.450
	32CB	32CA	310	164.98
	32CB	32CA	31CA	126.49
	32CB	32CA	32CD	19.890
	320	32CA	31C	105.54
25	320	32CA	32CG	124.05
	320	32CA	310	82.830
	320	32CA	31CA	115.83
	320	32CA	32CD	122.48
	31C	32CA	32CG	129.49
30	31C	32CA	310	26.280
	31C	32CA	31CA	12.250
	31C	32CA	32CD	131.65
	32CG	32CA	310	145.52
~ -	32CG	32CA	31CA	120.06
35	32CG	32CA	32CD	13.440
	310	32CA	31CA	38.530
	310	32CA	32CD	153.77
	31CA	32CA	32CD	120.38
40	32CG	32CB	32CA	115.02
40	32CG	32CB	32N	109.57
	32CG	32CB	32C	143.75

32CG

32CG

32CB

32CB

32CD

32NE

34.150

54.870

PCT/US02/38715

	32CG	32CB	320	130.87
	32CG	32CB	31C	112.55
	32CA	32CB	32N	33.480
	32CA	32CB	32C	35.450
5	32CA	32CB	32CD	148.24
	32CA	32CB	32NE	161.45
	32CA	32CB	320	44.220
	32CA	32CB	31C	25.510
	32N	32CB	32C	58.870
10	32N	32CB	32CD	130.02
	32N	32CB	32NE	157.91
	32N	32CB	320	74.310
	32N	32CB	31C	8.050
	32C	32CB	32CD	169.75
15	32C	32CB	32NE	143.17
	32C	32CB	320	19.650
	32C	32CB	31C	51.900
	32CD	32CB	32NE	28.390
	32CD	32CB	320	150.28
20	32CD	32CB	31C	136.44
	32NE	32CB	320	127.38
	32NE	32CB	31C	164.81
	320	32CB	31C	.66.560
	32CB	32CG	32CD	111.80
25	32CB	32CG	32NE	95.320
	32CB	32CG	32CA	32.520
	32CB	32CG	32N	44.590
	32CB	32CG	32CZ	94.360
	32CB	32CG	32C	22.610
30	32CD	32CG	32NE	32.100
	32CD	32CG	32CA	143.52
	32CD	32CG	32N	135.66
	32CD	32CG	32CZ	25.790
	32CD	32CG	32C	133.10
35	32NE	32CG	32CA	125.96
	32NE	32CG	32N	137.03
	32NE	32CG	32CZ	8.900
	32NE	32CG	32C	110.60
	32CA	32CG	32N	24.970
40	32CA	32CG	32CZ	126.39
	32CA	32CG	32C	16.050
	32N	32CG	32CZ	132.81
	32N	32CG	32C	39.010

WO 03/048733	PCT/US02/38715

	32CZ	32CG	32C	112.09
	32NE	32CD	32CG	114.11
	32NE	32CD	32CZ	26.540
	32NE	1 32CD	32CB	96.240
5	32NE	32CD	32NH1	54.560
	32NE	32CD	32NH2	16.130
	32NE	32CD	32CA	105.65
	32CG	. 32CD	32CZ	138.57
	, 32CG	32CD	32CB	34.050
10	32CG	32CD	32NH1	159.55
	32CG	32CD	32NH2	129.25
	32CG	32CD	32CA	23.040
	32CZ	32CD	32CB	112.59
	32CZ	32CD	32NH1	28.030
15	32CZ	32CD	32NH2	10.410
	32CZ	32CD	32CA	123.99
	32CB	32CD	32NH1	125.78
	32CB	32CD	32NH2	106.62
	32CB	32CD	32CA	11.860
20	32NH1	32CD	32NH2	38.430
	32NH1	32CD	32CA	137.27
	32NH2	32CD	32CA	117.35
	32CZ	32NE	32CD	124.08
	32CZ	32NE	32NH1	29.780
25	32CZ	32NE	32NH2	29.640
	32CZ	32NE	32CG	154.12
	32CZ	32NE	32CB	139.34
	32CD	32NE	32NH1	94.300
	32CD	32NE	32NH2	153.72
30	32CD	32NE	32CG	33.790
	32CD	32NE	32CB	55.370
	32NH1	32NE	32NH2	59.420
	32NH1	32NE	32CG	125.76
	32NH1		32CB	124.83
35	32NH2	32NE	32CG	168.08
	32NH2	32NE	32CB	138.50
	32CG	32NE	32CB	29.800
	32NH2	32CZ	32NH1	119.18
	32NH2	32CZ	32NE	120.54
40	32NH2	32CZ	32CD	149.91
	32NH2	32CZ	32CG	135.63
	32NH1	32CZ	32NE	120.28
	32NH1	32CZ	32CD	90.900
				452

WO 03/048733	PCT/US02/38715

	•			
	32NH1	32CZ	32CG	104.70
	32NE	32CZ	, 32CD	29.380
	32NE	32CZ	32CG	16.970
	32CD	32CZ	32CG	15.640
5	32CZ	32NH1	32NH2	30.400
	32CZ	32NH1	. 32NE	29.940
	32CZ	32NH1	32CD	61.070
	32NH2	. 32NH1	32NE	60.340
	32NH2	32NH1	32CD	91.470
10	32NE	, 32NH1	32CD	31.130
	32CZ	32NH2	32NH1	30.420
	32CZ	32NH2	32NE	29.820
	32CZ	32NH2	32CD	19.680
	32NH1	32NH2	32NE	60.240
15	32NH1	32NH2	32CD	50.090
	32NE	32NH2	32CD	10.140
	320	32C	32CA	120.36
	320	32C	32N	143.86
	320	32C	32CB	117.16
20	320	32C	. 310	106.87
	320	32C	31C	130.20
	320	32C	32CG	109.42
	320	32C	290	156.25
	32CA	32C	32N	34.330
25	32CA	32C	32CB	35.530
	32CA	32C	310	70.870
	32CA	32C	31C	55.810
	32CA	32C	32CG	27.830
	32CA	32C	290	80.940
30	32N	32C	32CB	59.960
	32N	32C	310	49.410
	32N	32C	31C	26.640
	32N	32C	32CG	58.700
	32N	32C	290	59.800
35	32CB	32C	310	105.44
	32CB	32C	31C	86.190
	32CB	32C	32CG	13.640
	32CB	32C	290	73.110
	310	32C	31C	24.410
40	310	32C	32CG	98.470
	310	32C	290	89.350
	31C	32C	32CG	82.980
	31C	32C	290	69.110

WO 03/048733	PCT/US02/38715

	32CG	32C	290	84.420
	32C	320	32CA	33.440
	32C	320	32CB	43.190
	32C.	320	310	53.140
5	32C	320	32N	24.230
	32C	320	31C	35.710
	32CA	320	32CB	26.510
•	32CA	320	310	53.330
	32CA	320	32N	18.820
10	32CA	320	31C	37.570
	32CB	320	310	79.570
	32CB	320	32N	42.650
	32CB	320	31C	62.750
	310	320	32N	37.890
15	310	320	31C	18.340
	32N	320	31C	20.180
	45CA	45N	45C	35.410
	45CA	45N	45CB	35.970
	45CA	45N	45CG	57.760
20	45CA	45N	450	31.000
	45CA	45N	45ND1	77.420
	45CA	45N	45CD2	60.650
	45C	45N	45CB	62.400
	45C	45N	45CG	90.430
25	45C	45N	450	11.620
	45C	45N	45ND1	106.60
	45C	45N	45CD2	96.040
	45CB	45N	45CG	30.090
	45CB	45N	450	63.510
30	45CB	45N	45ND1	44.300
	45CB	45N	45CD2	45.110
	45CG	45N	450	88.630
	45CG	45N	45ND1	21.500
	45CG	45N	45CD2	20.440
35	450	45N	45ND1	107.35
	450	45N	45CD2	90.420
	45ND1	45N	45CD2	34.960
	45N	45CA	45C	110.71
	45N	45CA	45CB	110.04
40	45N	45CA	450	130.63
	45N	45CA	45CG	92.950
	45N	45CA	45CD2	96.020
	45N	45CA	45ND1	79.230
				455

WO 03/048733	•	PCT/US02/38715
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	45N	45CA	300D1	102.51
	45C	45CA	45CB	112.68
	. 45C	45CA	450	26.040
	45C	45CA	45CG	145.56
5	45C	45CA	45CD2	153.21
	45C	45CA	45ND1	144.96
	45C	45CA	300D1	115.68
	45CB	45CA	450	111.13
	45CB	45CA	45CG	33.260
10	45CB	45CA	45CD2	53.130
	45CB	45CA	45ND1	36.450
	45CB	45CA	300D1	104.60
	450	45CA	45CG	136.10
	450	45CA	45CD2	130.56
15	450	45CA	45ND1	147.24
	450	45CA	300D1	92.340
	45CG	45CA	45CD2	23.730
	45CG	45CA	45ND1	16.650
	45CG	45CA	300D1	81.150
20	45CD2	45CA	45ND1	36.970
	45CD2	45CA	300D1	57.490
	45ND1	45CA	300D1	93.340
	45CG	45CB	45CA	112.60
	45CG	45CB	45N	94.770
25	45CG	45CB	45ND1	27.280
	45CG	45CB	45C	145.67
	45CG	45CB	45CD2	23.270
	45CG	45CB	450	142.79
	45CG	45CB	45CE1	13.750
30	45CG	45CB	45NE2	7.790
	45CA	45CB	45N	33.990
	45CA	45CB	45ND1	122.45
	45CA	45CB	45C	33.450
	45CA	45CB	45CD2	98.710
35	45CA	45CB	450	42.910
	45CA	45CB	45CE1	116.52
	45CA	45CB	45NE2	106.57
	45N	45CB	45ND1	93.090
	45N	45CB	45C	58.720
40	45N	45CB	45CD2	92.950
	45N	45CB	450	74.290
	45N	45CB	45CE1	92.170
	45N	45CB	45NE2	92.100
	•			156

WO 03/048733	PCT/US02/38715
WO 03/048733	PC1/US02/38/1

	· · · · · · · · · · · · · · · · · · ·			
	45ND1	45CB	45C	151.55
	45ND1	45CB	45CD2	50.470
	45ND1	. 45CB	450	164.62
	45ND1	45CB	45CE1	13.790
5	45ND1	45CB	45NE2	34.610
	45C	45CB	45CD2	127.91
	45C	45CB	450	19.560
	45C	45CB	45CE1	149.49
	45C	45CB	45NE2	138.98
10	45CD2	45CB	450	120.15
	45CD2	45CB	45CE1	36.740
	45CD2	45CB	45NE2	15,920
	450	45CB	45CE1	153.86
	450	45CB	45NE2	135.00
15	45CE1	45CB	45NE2	20.840
	45CD2	45CG	45ND1	106.01
	45CD2	45CG	45CB	130.89
	45CD2	45CG	45NE2	36.670
	45CD2	45CG	45CE1	71.600
20	45CD2	, 45CG	45CA	107.89
•	45CD2	45CG	45N	109.57
	45CD2	45CG	45C	115.29
	45ND1	45CG	45CB	122.88
	45ND1	45CG	45NE2	69.340
25	45ND1	45CG	45CE1	34.420
	45ND1	45CG	45CA	131.79
	45ND1	45CG	45N	106.27
	45ND1	45CG	45C	132.76
	45CB	45CG	45NE2	166.91
30	45CB	45CG	45CE1	156.97
	45CB	45CG	45CA	34.140
	45CB	45CG	45N	55.140
	45CB	45CG	45C	21.710
	45NE2	45CG	45CE1	34.920
35	45NE2	45CG	45CA	135.17
	45NE2	45CG	45N	119.59
	45NE2	45CG	45C	146.62
	45CE1	45CG	45CA	146.63
	45CE1	45CG	45N	117.91
40	45CE1	45CG	45C	156.80
	45CA	45CG	45N	29.290
	45CA	45CG	45C	12.800
	45N	45CG	45C	39.250
				457

	WO 03/048733				PCT/US02/38715
	45CG	45CD2	45NE2	107.24	
	45CG	45CD2	45ND1	37.350	
	45CG	45CD2	45CE1	72.490	
	45CG	45CD2	45CB	25.840	
5	45CG	45CD2	45CA	48.370	
	45CG	45CD2	300D1	117.87	
	45CG	45CD2	30CB	117.20	
	· 45CG	. 45CD2	45N	49.990	
	45CG	45CD2	30CG	120.03	
10	45NE2	45CD2	45ND1	69.890	
	45NE2	45CD2	45CE1	34.750	
	45NE2	45CD2	45CB	13290	
	45NE2	45CD2	45CA	141.09	
	45NE2	45CD2	300D1	126.04	•
15	45NE2	45CD2	30CB	94.760	$(\mathbf{x}_{i},\mathbf{x}_{i},\mathbf{x}_{i}) = \mathbf{x}_{i} + \mathbf{x}_{i} + \mathbf{x}_{i}$
	45NE2	45CD2	45N	118.90	•
	45NE2	45CD2	30CG	112.54	•
	45ND1	45CD2	45CE1	35.150	

45CB

45CA

300D1

30CB

. 45N.

30CG

45CA

300D1

30CB

45N

30CG

45CA

300D1

30CB

30CG

300D1

30CB

45N

30CG

30CB

45N

30CG

45N

45N

45CB

63.110

81.050

71, 340

146.78

120.56

137.77

112.51

150.32

111.11

133.23

95.890

28.160

94.020

41.950

69.640

77.970

23.330

72.900

39.260

75.610

17.090

67.700

105.83

100.29

98.210

45CD2

45ND1

45ND1

45ND1

45ND1

4.5ND1

45ND1

45CE1

45CE1

45CE1

45CE1

45CE1

45CE1

45CB

45CB

45CB

45CB

45CB

45CA

45CA

45CA

45CA

300D1

300D1

300D1

30CB

20

25

30

35

40

458

	WO 03/048733			
	30CB	45CD2	30CG	22.180
	45N	45CD2	30CG	71.680
	45CE1	45ND1	45CG	109.46
•	45CE1	45ND1	45NE2	35.790
5	45CE1	45ND1	45CD2	72.830
	45CE1	45ND1	45CB	139.12
	45CE1	45ND1	45CA	128.17
	45CE1	45ND1	45N	121.97
	45CG	45ND1	45NE2	73.670
10	45CG	45ND1	45CD2	36.640
	45CG	45ND1	45CB	29.840
	45CG	45ND1	45CA	31.560
	45CG	45ND1	45N	52.230
	45NE2	45ND1	45CD2	37.030
15	45NE2	45ND1	45CB	103.39
	45NE2	45ND1	45CA	95.840
	45NE2	45ND1	45N	99.290
	45CD2	45ND1	45CB	66.410
	45CD2	45ND1	45CA	61.990
20	45CD2	45ND1	45N	73.700
	45CB	45ND1	45CA	21.110
	45CB	45ND1	45N	42.610
	45CA	45ND1	45N	23.350
	45NE2	45CE1	45ND1	108.40
25	45NE2	45CE1	45CD2	36.370
	45NE2	45CE1	45CG	72.280
	45NE2	45CE1	45CB	81.380
	45ND1	45CE1	45CD2	72.030
	45ND1	45CE1	45CG	36.120
30	45ND1	45CE1	45CB	27.090

45CE1

45CE1

45CE1

45NE2

45CG

45CB

45CB

45CD2

45ND1

45CG

45CB

45CG

45CB

45CB

45CB

45CG

45ND1

35.910

45.040

108.88

35.810

72.800

77.770

73.070

36.090

31.180

36.990

42.000

5.290

9.280

45CD2

45CD2

45CE1

45CE1

45CE1

45CE1

45CD2

45CD2

45CD2

45ND1

45ND1

45CG

35 .

40

45CG

459

	TNO 02/040822			
	WO 03/048733			
	450	45C	45CA	120.88
	450	45C	45N	144.55
	450	45C	45CB	116.29
	450	45C	48N	59.440
5	450	45C	45CG	116.81
	45CA	45C	45N	33.880
	45CA	45C	45CB	33.870
	45CA	, 45C	48N	105.56
	45CA	45C	45CG	21.630
10	45N	45C	45CB	58.880
	45N	45C	48N	97.930
	45N	45C	45CG	50.330
	45CB	45C	48N	135.29
	45CB	45C	45CG	12.620
15	48N	45C	45CG	123.54
	45C ,	450	45CA	33.070
	45C	450	49N	151.39
	45C	450	48N	100.94
	45C	450	45CB	44.150
20	45C	450	45N	23.830
	45C	450	48CA	117.88
	45C	450	48C	140.93
	. 45C	450	49CB	145.57
	45C	450	49CA	159.39
25	45CA	450	49N	146.88
	45CA	450	48N	99.460
	45CA	450	45CB	25.960
	45CA	450	45N	18.370
	45CA	450	48CA	104.05
30	45CA	450	48C	127.00
	45CA	450	49CB	171.68
	45CA	450	49CA	163.08
	4 9 N	450	48N	53.030
	49N	450	45CB	157.31
35	49N	450	45N	139.95
	49N	450	48CA	43.090
	49N	450	48C	19.950
	4 9 N	450	49CB	40.320
	49N	450	49CA	18.350
40	48N	450	45CB	124.49
	48N	450	45N	87.380
	48N	450	48CA	24.280
	48N	450	48C	40.620

	WO 03/048733			
	48N	450	49CB	88.850
	48N	450	49CA	70.540
	45CB	450	45N	42.200
	45CB	450	48CA	123.39
5	45CB	450	48C	141.10
	45CB	450	49CB	145.86
	45CB	450	49CA	155.67
	45N	450	48CA	98.390
	45N	450	48C	122.61
10	45N	450	49CB	165.95
	45N	450	49CA	157.92
	48CA	450	48C	24.220
	48CA	450	49CB	83.390
	48CA	450	49CA	61.180
15	48C	450	49CB	59.910
	48C	450	49CA	37.310
	49CB	450	49CA	22.740
	48CA	48N	48C	36.480
	48CA	48N	49N	63.070
20	48CA	48N	450	93.220
	48CA	48N	480	32.330
	48CA	48N	45C	107.30
	48C	48N	49N	29.480
•	48C	48N	450	81.700
25	48C	48N	480	12.410
	48C	48N	45C	101.11
	49N	48N	450	60.320
	4 9 N	48N	480	40.670
	49N	48N	45C	79.480
30	450	48N	480	93.900
	450	48N	45C	19.610
	480	48N	45C	113.14
٠	48N	48CA	48C	108.79
~ ~	48N	48CA	480	128.65
35	. 48N	48CA	49N	84.880
,	48N	48CA	450	62.500
	48N	48CA	49CA	92.330
,	48C	48CA	480	26.840
40	48C	48CA	49N	29.300
40	48C	48CA	450	83.150
	48C	48CA	49CA	19.890
	480	48CA	49N	56.140

48CA

480

461

108.36

450

WO 03/048733		PCT/US02/38715
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	480	48CA	49CA	46.710
	49N	48CA	450	56.090
	49N	48CA	49CA	9.430
	450	48CA	49CA	64.890
5	480	48C	49N	123.25
	480	48C	48CA	119.60
•	480	48C	48N	142.82
	480	48C	49CA	92.400
	480	48C	49C	77.160
10	480	48C	450	158.07
	480	48C	49CB	107.61
	480	48C	490	62.950
	49N	48C	48CA	117.14
	49N	48C	48N	88.270
15	49N	48C	49CA	30.850
	49N	48C	49C	52.700
	49N	48C	450	48.910
	49N	48C	49CB	15.740
	49N	48C	490	64.070
20	48CA	48C	48N	34.730
	48CA	48C	49CA	147.97
	48CA	48C	49C	149.29
,	48CA	48C	450	72.630
	48CA	48C	49CB	132.78
25	48CA	48C	490	158.92
	48N	48C	49CA	116.79
	48N	48C	49C	116.29
	48N	48C	450	57.670
	48N	48C	4 9CB	103.52
30	48N	48C	490	129.63
	49CA	48C	49C	30.400
	49CA	48C	450	77.590
	49CA	48C	49CB	15.360
	49CA	48C	490	36.590
35	49C	48C	450	101.29
	49C	48C	49CB	41.610
	49C	48C	490	14.690
	450	48C	49CB	62.570
	450	48C	490	112.91
40	49CB	48C	490	50.700
	48C	480	49N	29.620
	48C	480	48CA	33.560
	48C	480	49CA	61.300
				462

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	48C	480	52N	152.10
	48C	480	49C	79.110
	48C	480	48N	24.770
	48C	480	490	98.710
5	48C	480	52CB	144.86
	48C	480	52CA	158.77
	49N	480	48CA	63.180
	49N	480	49CA	31.680
	49N	480	52N	131.03
10	49N	480	49C	53.300
	49N	480	48N	51.490
	49N	480	490	71.410
	49N	480	52CB	117.10
	49N	480	52CA	129.65
15	48CA	480	49CA	94.860
	48CA	480	52N	149.04
	48CA	480	49C	108.83
	48CA	480	48N	19.010
	48CA	480	490	128.77
20	48CA	480	52CB	165.82
	48CA	480	52CA	165.56
	49CA	480	52N	102.95
	49CA	480	49C	30.500
	49CA	480	4811	81.880
25	49CA	480	490	43.260
	49CA	480	52CB	86.590
	49CA	480	52CA	98.140
	52N	480	49C	77.730
	52N	480	48N	140.98
30	52N	480	490	60.200
	52N	480	52CB	42.620
	52N	480	52CA	19.450
	49C	480	48N	90.800
	49C	480	490	20.000
35	49C	480	52CB	79.260
	49C	480	52CA	80.050
	48N	480	490	110.46
	48N	480	52CB	168.46
	48N	480	52CA	159.96
40	490	480	52CB	60.150
	490	480	52CA	60.240
	52CB	480	52CA	23.440
	48C	4 9 N	49CA	121.24
				463

WO 03/048733	PCT/US02/38715
WO 03/048/33	PC 1/USU2/38/15

•	48C	49N	480	27.130
	48C	49N	, 48CA	33.560
	48C	4 9 N	49C	101.49
	48C	4 9 N	49CB	155.88
5	48C	49N	48N	62.250
	48C	49N	450	111.14
	48C	49N	49CG	146.47
	48C	· 49N	490	95.860
	49CA	49N	480	94.120
10	49CA	49N	48CA	154.78
	49CA	4 9N	49C	36.270
	49CA	49N	49CB	34.930
	4 9CA	49N	48N	160.92
	49CA	49N	450	122.27
15	49CA	49N	49CG	45.130
	49CA	49N	490	32.710
	480	49N	48CA	60.680
	480	49N	49C	78.740
	480	49N	49CB	128.86
20	480	49N	48N	87.840
	480	49N	450	134.73
	480	49N	49CG	126.47
	480	49N	490	70.850
	48CA	49N	49C	127.76
25	48CA	49N	49CB	170.15
	48CA	49N	48N	32.050
	48CA	49N	450	80.820
	48CA	49N	49CG	151.39
	48CA	49N	490	126.10
30	49C	49N	49CB	60.860
	49C	49N	48N	126.57
	49C	49N	450	146.51
	, 49C	49N	49CG	79.150
	49C	49N	490	12.200
35	49CB	49N	48N	140.85
	49CB	49N	450	89.520
	49CB	49N	49CG	23.940
	4 9CB	49N	490	63.430
	48N	49N	450	66.650
40	48N	49N	49CG	142.91
	48N .	49N	490	133.25
٠	450	49N	49CG	77.820
	450	49N	490	152.81
	•			464

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49CG	49N	490	77.780	

	49CG	49N	490	77.780
	4 9 N	49CA	49C	109.24
	4 9N	49CA	49CB	111.98
•	4 9 N	49CA	490	128.08
5	49N	49CA	48C	27.910
	4 9N	49CA	49CG	111.32
	4 9N	49CA	480	54.200
	4 9N	49CA	48CA	15.790
	4 9N	49CA	450	39.390
10	49C	49CA	49CB	109.06
	49C	49CA	490	26.050
	49C	49CA	48C	95.730
	4 9C	49CA	49CG	132.71
	49C	49CA	480	82.190
15	49C	49CA	48CA	101.41
	49C	49CA	450	137.56
	49CB	49CA	490	109.97
	49CB	49CA	48C	139.72
	49CB	49CA	49CG	31.740
20	49CB	49CA	480	165.37
	49CB	49CA	48CA	127.74
	49CB	49CA	450	75.350
	490	49CA	48C	106.16
b.	490	49CA	49CG	120.47
25	490	49CA	480	84.290
	490	49CA	48CA	115.68
	490	49CA	450	163.33
	48C	49CA	49CG	131.14
	48C	49CA	480	26.290
30	48C	49CA	48CA	12.140
	48C	49CA	450	65.100
	4 9CG	49CA	480	142.54
	49CG	49CA	48CA	123.44
0.5	49CG	49CA	450	72.630
35	480	49CA	48CA	38.430
	480	49CA	450	90.040
	48CA	49CA	450	53.930
	49CG	49CB	49CA	116.24
40	49CG	49CB	49N	114.58
40	49CG	4 9CB	49C	141.15
	49CG	49CB	49SD	36.600
	49CG	49CB	490	126.24
,	49CG	49CB	49CE	53.680
				465

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	49CG	49CB	48C	114.27
	49CG	49CB	450	85.220
	49CA	49CB	49N	33.090
	49CA	4 9CB	49C	35.390
5	49CA	49CB	49SD	148.81
	49CA	49CB	490	43.790
	49CA	49CB	49CE	162.24
	49CA	49CB	48C	24.910
	49CA	49CB	450	81.910
10	49N	49CB	49C	58.660
	4 9 N	49CB	49SD	148.76
	4 9 N	49CB	490	73.620
	4 9N	49CB	49CE	132.71
	49N	49CB	48C	8.380
15	4 9N	49CB	450	50.170
	49C	49CB	49SD	147.78
	49C	49CB	490	19.360
	49C	49CB	49CE	161.28
	49C	49CB	48C	53.120
20	49C	49CB	450	107.23
	49SD	49CB	490	129.07
	49SD	49CB	49CE	31.240
	49SD	49CB	48C	150.42
	49SD	49CB	450	104.41
25	490	49CB	49CE	153.30
	490	49CB	48C	66.660
	490	49CB	450	123.72
	49CE	49CB	48C	139.97
	49CE	49CB	450	82.570
30	48C	49CB	450	57.520
	49CB	49CG	49SD	113.95
	49CB	49CG	49CA	32.020
	49CB	49CG	49CE	99.440
	49CB	49CG	49N	41.480
35	49CB	49CG	49C	24.300
	49SD	49CG	49CA	142.90
	49SD	49CG	49CE	38.850
*	49SD	49CG	49N	152.35
	49SD	49CG	49C	126.30
40	49CA	49CG	49CE	129.70
	49CA	49CG	49N	23.540
	49CA	49CG	49C	17.180
	49CE	49CG	49N	120.53
	•			466

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	49CE	4 9CG	49C	122.67
	49N	49CG	49C	39.050
	49CE	49SD	49CG	98.910
	4 9CE	49SD	49CB	90.350
5	49CG	49SD	49CB	29.450
	49SD	49CE	49CG	42.240
	49SD	49CE	49CB	58.410
	49CG	. 49CE	49CB	26.880
	490	49C	4 9CA	120.82
10	490	49C	49N	142.98
	490	49C	49CB	118.34
	490	49C	480	103.81
	490	49C	48C	126.98
	490	49C	52N	58.820
15	490	49C	49CG	107.87
	49CA	49C	49N	34.490
	49CA	49C	49CB	35.550
	49CA	49C	480	67.310
	49CA	49C	48C	53.870
20	49CA	49C	52N	110.05
	49CA	49C	4 9CG	30.110
	49N	49C	4 9CB	60.480
	49N	49C	480	47.960
	49N	49C	48C	25.810
25	49N	49C	52N	98.720
	4 9 N	49C	4 9CG	61.800
	49CB	49C	480	102.42
	49CB	49C	48C	
	49CB	49C	52N	142.85
30	49CB	49C	49CG	14.550
	480	49C	48C	23.740
	480	49C	52N	50.760
	480	49C	4 9CG	96.450
25	48C	49C	52N	73.810
35	48C	49C	49CG	83.800
	52N	49C	49CG	129.66
	49C	490	49CA	33.120
	49C	490	4 9CB	42.300
40	49C	490	52N	102.39
40	49C	490 490	480	56.180
	49C		49N	24.820
	49C	490 490	52CB 52CA	115.92 120.50
	49C	490	JZCA	
				467
				•.

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	49C	490	52C	141.89
	49C	490	48C	38.330
	49CA	490	49CB	26.240
	49CA	4 90	52N	103.66
5	49CA	490	480	52.450
	49CA	490	49N	19.220
	49CA	490	52CB	94.190
	49CA	490	52CA	110.37
	49CA	490	52C	132.79
10	49CA	490	48C	37.250
	49CB	490	52N	129.79
	49CB	490	480	78.650
	49CB	490	49N	42.950
	49CB	490	52CB	111.70
15	49CB	490	52CA	132.78
	49CB	490	52C	150.79
	49CB	490	48C	62.640
	52N	490	480	51.750
	52N	490	49N	89.230
20	52N	490	52CB	42.290
	52N	490	52CA	23.070
	52N	490	52C	39.550
	52N	490	48C	, 69.220
	480	490	49N	37.740
25	480	490	52CB	62.180
	480	490	52CA	64.870
	480	490	52C	87.820
	480	490	48C	18.340
	4 9 N	490	52CB	92.020
30	4 9N	490	52CA	101.56
	4 9 N	490	52C	124.93
	49N	490	48C	20.070
	52CB	490	52CA	24.340
	52CB	490	52C	39.750
35	52CB	490	48C	78.350
	52CA	490	52C	23.400
	52CA	490	48C	83.190
	52C	490	48C	106.15
	52CA	52N	52C	36.160
40	52CA	52N	52CB	35.020
	52CA	52N	480	118.11
	52CA	52N	490	95.590
	52CA	52N	520	34.260
				4.60

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	52CA	52N	49C	110.60
	52CA	52N	52CG	22.800
	52C	52N	52CB	61.280
	52C	52N	480	138.59
5	52C	52N	490	81.420
	52C	52N	520	13.660
	52C	52N	49C	100.20
	52C	52N	52CG	52.160
	52CB	52N	480	83.850
10	52CB	52N	490	75.680
	52CB	52N	520	65.820
	52CB	52N	49C	84.150
	52CB	52N	52CG	12.280
	480	52N	490	68.050
15	480	52N	520	148.48
	480	52N	49C	51.510
	480	52N	52CG	95.630
	490	52N	520	95.050
	490	52N	49C	18.790
20	490	52N	52CG	83.320
	520	52N	49C	113.83
	520	52N	52CG	54.830
	49C	52N	52CG	94.170
	52N	52CA	52C	109.25
25	52N	52CA	52CB	112.09
	52N	52CA	520	125.56
	52N	52CA	52CG	144.63
	52N	52CA	52CD1	150.46
	52N	52CA	490	61.340
30	52N	52CA	480	42.440
	52N	52CA	52CD2	131.15
	52C	52CA	52CB	110.05
	52C	52CA	520	26.420
	52C	52CA	52CG	92.510
35	52C	52CA	52CD1	100.27
	52C	52CA	490	80.610
	52C	52CA	480	134.08
	52C	52CA	52CD2	101.02
	52CB	52CA	520	113.90
40	52CB	52CA	52CG	32.610
	52CB	52CA		56.390
	52CB	52CA		73.420
	52CB	52CA	480	70.630
				460

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	52CB	52CA	52CD2	19.210	
	520	52CA	, 52CG	85.830	
	520	52CA	52CD1	81.620	
	520	52CA	490	106.77	
5	520	52CA	480	160.23	
	520	52CA	52CD2	98.070	
	52CG	52CA	52CD1	30.440	
	52CG	52CA	490	96.880	
	52CG	52CA	480	102.57	
10	52CG	52CA	52CD2	13.480	
	52CD1	52CA	490	127.05	
•	52CD1	52CA	480	114.61	•
	52CD1	52CA	52CD2	39.470	
	490	52CA	480	54.890	
15	490	52CA	52CD2	87.930	
	480	52CA	52CD2	89.170	
	52CA	. 52CB	52CG	114.81	•
	52CA	52CB	52N	32.900	
	52CA	52CB	52C	34.650	
20	52CA	52CB ·	52CD1	92.870	,
	52CA	52CB	52CD2	149.21	
	52CA	52CB	520	40.980	
	. 52CA .	52CB	. 490	82.240	atherine and are accounted to the contract of
	52CA	52CB	480	85.930	•
25	52CG	52CB	52N	147.64	
	52CG	52CB	52C	95.470	. •
	52CG	52CB	52CD1	34.840	
	52CG	52CB	52CD2	34.490	·
	52CG	52CB	520	79.430	
30	52CG	52CB	490	133.14	
	52CG	52CB	480	156.22	
	52N	52CB	52C	58.130	· ·
	52N	52CB	52CD1	120.49	
	52N	52CB	52CD2	176.02	
35	52N	52CB	520	71.010	
	52N	52CB	490	62.030	
	52N	52CB	480	53.530	
	52C	52CB	52CD1	91.890	•
	52C	52CB	52CD2	125.58	
40	52C	52CB	520	18.270	
	52C	52CB	490	74.080	
	52C	52CB	480	108.30	
	52C 52CD1	52CB 52CB	480 52CD2	108.30 59.460 470	

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	52CD1	52CB	520	73.720
	52CD1	52CB	490	161.73
	52CD1	52CB	480	139.85
·	52CD2	52CB	520	112.23
5	52CD2	52CB	490	119.44
	52CD2	52CB	480	123.55
	520	52CB	490	91.500
	520	52CB	480	123.93
	490	52CB	480	57.670
10	52CD1	52CG	52CD2	109.75
	52CD1	52CG	52CB	109.89
	52CD1	52CG	52CA	89.960
	52CD1	52CG	52C	97.850
	52CD1	52CG	520	83.370
15	. 52CD1 ,	52CG	52N	97.080
•	52CD2	52CG	52CB	110.66
	52CD2	52CG	52CA	143.17
	52CD2	52CG	52C	152.23
	52CD2	52CG	520	162.30
20	52CD2	52CG	52N	130.60
	52CB	52CG	52CA	32.590
	52CB	52CG	52C	54.470
•	52CB	52CG	520	74.040
	52CB	52CG	52N	20.080
25	52CA	52CG	52C	29.630
	52CA	52CG	520	44.400
	52CA	52CG	52N	12.570
	52C	52CG	520	21.080
	52C	52CG	52N	38.700
30	520	52CG	52N	55.970
	52CG	52CD1	52CD2	35.160
	52CG	52CD1	52CB	35.270
	52CG	52CD1	52CA	59.600
	52CG	52CD1	520	71.410
35	52CG	52CD1	52C	57.360
	52CD2	52CD1	52CB	60.550
	52CD2	52CD1	52CA	90.490
	52CD2	52CD1	520	105.83
	52CD2	52CD1	52C	92.480
40	52CB	52CD1	52CA	30.740
	52CB	52CD1	520	63.610
	52CB	52CD1	52C	43.990
	52CA	52CD1	520	41.470
				<i>4</i> 71

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	52CA	52CD1	52C	24.450
	520	52CD1	52C	19.680
	52CG	52CD2	52CD1	35.090
	52CG	52CD2	52CB	34.850
5	52CG	52CD2	52CA	23.350
	52CD1	52CD2	52CB	59.990
	52CD1	52CD2	52CA	50.040
	52CB	52CD2	52CA	11.580
	520	52C	52CA	120.16
10	520	52C	52N	138.43
	520	52C	52CB	121.83
	520	52C	52CG	94.760
	520	52C	52CD1	77.910
	520	52C	490	162.23
15	52CA	52C	52N	34.590
	52CA	52C	52CB	35.300
•	52CA	52C	52CG	57.870
	52CA	52C	52CD1	55.280
	52CA	52C	490	75.990
20	52N	52C	52CB	60.600
	52N	52C	52CG	89.150
	52N	52C	52CD1	89.870
i	52N	52C	490	
	52CB	52C	52CG	30.060
25	52CB	52C	52CD1	44.120
	52CB	52C	490	66.170
	52CG	52C	52CD1	24.790
	52CG	52C	490	88.000
	52CD1	52C	490	109.46
30	52C	520	52CA	33.420
	52C	520	52CB	39.900
	52C	520	52CG	64.160
	52C	520	52N	27.900
0.5	52C	520	52CD1	82.410
35	52CA	520	52CB	25.130
	52CA	520	52CG	49.770
	52CA	520	52N	20.180
	52CA	520	52CD1	56.910
40	52CB	520	52CG	26.530
40	52CB	520	52N	43.170
	52CB	520	52CD1	42.670
	52CG	520	52N	69.200
	52CG	520	52CD1	25.220

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	52N	520	52CD1	76.680
	70CA	70N	70CB	37.460
	70CA	70N	[*] 70C	35.750
	70CA	70N	700	55.180
5	70CA	70N	71N	35.970
	70CA	70N	. 70CG	27.370
	70CB	70N	70C	62.020
ě	70CB	70N	700	67.000
	70CB	70N	71N	70.330
10	70CB	70N	70CG	10.490
	70C	70N	700	24.900
	70C	70N	71N	17.080
	70C	70N	70CG	55.470
*	700	70N	71N	40.450
15	700	70N	70CG	64.880
•	71N	70N	70CG	61.620
	70N	70CA	70CB	106.91
	70N	70CA	70C	110.27
	70N	70CA	700	94.920
20	70N	70CA	71N	123.39
*	70N	70CA	70CG	137.63
	70N	70CA	70CD1	150.73
	70N	70CA	70CD2	130.99
•	70N	70CA	71CA	120.25
25	70CB	70CA	70C	109.97
	70CB	70CA	700	95.430
	70CB	70CA	71N	121.60
	70CB	70CA	70CG	31.050
	70CB	70CA	70CD1	54.880
30	70CB	70CA	70CD2	25.460
	70CB	70CA	71CA	118.53
	70C	70CA	700	26.590
	70C	70CA	71N	29.160
	70C	70CA	70CG	96.100
35	70C	70CA	70CD1	98.220
	70C	70CA	70CD2	90.820
	70C	70CA	71CA	20.220
	700	70CA	71N	55.750
	700	70CA	70CG	94.790
40	700	70CA	70CD1	108.55
	700	70CA	70CD2	84.990
	700	70CA	71CA	46.810
	71N	70CA	70CG	95.770
				473

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	71N	70CA	70CD1	85.040
	71N	70CA	70CD2	96.710
	71N	70CA	71CA	8.940
	70CG	7.0CA	70CD1	26.790
5	70CG	70CA	70CD2	12.590
	70CG	70CA	71CA	95.830
	70CD1	70CA	70CD2	38.940
	70CD1	· 70CA	71CA	88.910
	70CD2	70CA	71CA	94.810
10	70CG	70CB	70CA	117.56
	70CG	70CB	70N	152.70
	70CG	70CB	. 70C	100.55
١.	70CG	70CB	. 70CD2	28.640
	70CG	70CB	70CD1	28.170
15	70CG	70CB	700	106.07
	70CG	70CB	71N	87.340
	70CG	.70CB	70CE2	19.310
	70CG	70CB	70CE1	18.640
	70CA	70CB	70N	35.640
20	70CA	70CB	70C	35.040
	70CA	70CB	70CD2	139.47
	70CA	70CB	70CD1	95.650
	70CA ·	70CB	700	- 53.800
	70CA	70CB	71N	36.510
25	70CA	70CB	70CE2	134.74
	70CA	70CB	70CE1	105.29
	70N	70CB	70C	60.030
	70N	70CB	70CD2	168.48
	70N	70CB	70CD1	127.04
30	70N	70CB	700	64.910
	70N	70CB	71N	69.250
	70N	70CB	70CE2	170.05
	70N	70CB	70CE1	137.27
	70C	70CB	70CD2	110.54
35	70C	70CB	70CD1	92.340
	70C	70CB	700	24.450
	70C	70CB	71N	17.380
	70C	70CB .	70CE2	110.50
	70C	70CB	70CE1	98.260
40	70CD2	70CB	70CD1	56.640
	70CD2	70CB	700	103.72
	70CD2	70CB	71N	103.59
	70CD2	70CB	70CE2	10.040
			•	474

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	70CD2	70CB	70CE1	46.680
	70CD1	70CB	700	108.56
	70CD1	70CB	71N	75.480
	70CD1	70CB	70CE2	46.880
5	70CD1	70CB	70CE1	10.230
	7,00	70CB	71N	40.070
•	700	70CB	70CE2	107.98
	700	70CB	70CE1	111.25
	71N	70CB	70CE2	100.81
10	71N	70CB	70CE1	82.170
•	70CE2	70CB	70CE1	36.820
	70CD1	70CG	70CD2	118.06
	70CD1	70CG	70CB	121.18
	70CD1	70CG	70CE2	88.760
15	70CD1	70CG	70CE1	29.500
	70CD1	70CG	70CA	96.460
	70CD1	70CG	70CZ	59.020
	70CD1	70CG	70C	98.630
	70CD1	70CG	700	115.86
20	70CD1	70CG	71N	80.340
	70CD1	70CG	70N	106.78
	70CD2	70CG	70CB	120.20
	70CD2	70CG	70CE2	29.310
•	70CD2	70CG	70CE1	88.570
25	70CD2	70CG	70CA	143.55
	70CD2	70CG	70CZ	59.050
	70CD2	70CG	70C	125.91
	70CD2	70CG	700	108.07
	70CD2	70CG	71N	130.21
30	70CD2	70CG	70N	135.15
	70CB	70CG	70CE2	148.81
	70CB	70CG	70CE1	149.97
	70CB	70CG	70CA	31.380
	70CB	70CG	70CZ	171.65
35	70CB	70CG	70C	51.310
	70CB	70CG	700	50.730
	70CB	70CG	71N	68.810
	70CB	70CG	70N	16.810
Ť	70CE2	70CG	70CE1	59.270
40	70CE2	70CG	70CA	167.45
	70CE2	70CG	70CZ	29.740
	70CE2	70CG	70C	139.06
	70CE2	70CG	700	126.97
				475

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	70CE2	70CG	71N	130.33
	70CE2	70CG	, 70N	164.45
	70CE1	70CG	70CA	125.33
	70CE1	70CG	70CZ	29.530
5	70CE1	70CG	70C	120.26
	70CE1	70CG .	700	132.40
	70CE1	70CG	71N	100.25
	70CE1	70CG	70N	136.28
	70CA	70CG	70CZ	153.44
10	70CA	70CG	70C	28.840
	70CA	70CG	700	40.600
	70CA	70CG	71N	40.450
	70CA	70CG	70N	15.000
	70CZ	70CG	70C	136.67
15	70CZ	70CG	700	137.52
	70CZ	. 70CG	71N	118.53
	70CZ	70CG	70N	165.80
	70C	70CG	700	18.990
	70C	70CG	71N	20.040
20	70C	70CG	70N	39.910
	. 700	70CG	71N	35.520
	700	70CG	70N	45.860
	71N	70CG	70N	54.640
	70CG	70CD1	70CE1	121.21
25	. 70CG	70CD1	· 70CD2	30,980
	70CG	70CD1	70CZ	91.090
	70CG	70CD1	70CB	30.650
	70CG	70CD1	70CE2	60.970
	70CG	70CD1	70CA	56.760
30	70CG	70CD1	70C	58.990
	70CG	70CD1	700H	101.71
	70CG	70CD1	71N	78.140
	70CE1	70CD1	70CD2	90.240
	70CE1	70CD1	70CZ	30.130
35	70CE1	70CD1	70CB	151.11
	70CE1	70CD1	70CE2	60.240
	70CE1	70CD1	70CA	170.56
	70CE1	70CD1	70C	146.02
	70CE1	70CD1	700H	19.540
40	70CE1	70CD1	71N	131.69
	70CD2	70CD1	70CZ	60.120
	70CD2	70CD1	70CB	61.440
	70CD2	70CD1	70CE2	30.000
				100

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	70CD2	70CD1	70CA	87.180
	70CD2	70CD1	70C	83.720
	70CD2	70CD1	700H	70.760
•	70CD2	70CD1	71N	98.740
5	70CZ	70CD1	70CB	121.24
	70CZ	70CD1	70CE2	30.120
	70CZ	70CD1	70CA	146.25
4	70CZ	70CD1	70C	131.84
	70CZ	70CD1	700H	10.700
10	70CZ	70CD1	71N	131.06
•	70CB	70CD1	70CE2	91.290
	70CB	70CD1	70CA	29.480
	70CB	70CD1	70C	43.450
	70CB	70CD1	700H	131.64
15	70CB	70CD1	71N	63.770
	70CE2	70CD1	70CA	116.79
,	70CE2	70CD1	70C	108.68
	70CE2	70CD1	700H	40.770
	70CE2	70CD1	71N	117.73
20	70CA	70CD1	70C	24.590
	70CA	70CD1	700H	156.75
	70CA	70CD1	71N	40.160
	70C	70CD1	700H	139.51
•	70C	70CD1	71N	20.610
25	700H	70CD1	71N	134.22
	70CZ	70CE1	70CD1	119.14
	70CZ	70CE1	700H	30.030
	70CZ	70CE1	70CE2	29.880
	70CZ	70CE1	70CG	89.850
30	70CZ	70CE1	70CD2	59.730
	70CZ	70CE1	70CB	100.75
	70CD1	70CE1	700H	149.06
	70CD1	70CE1	70CE2	89.270
	70CD1	70CE1	70CG	29.290
35	70CD1	70CE1	70CD2	59.420
	70CD1	70CE1	70CB	18.660
	70OH	70CE1	70CE2	59.890
	70ОН	70CE1	70CG	119.81
	70OH	70CE1	70CD2	89.720
40	70OH	70CE1	70CB	130.48
	70CE2	70CE1	70CG	59.990
	70CE2	70CE1	70CD2	29.850
	70CE2	70CE1	70CB	70.960
				177

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	70CG	70CE1	70CD2	30.130
	70CG	70CE1	70CB	11.390
	70CD2	70CE1	70CB	41.200
	70CE2	70CD2	70CG	121.11
5	70CE2	70CD2	70CD1	90.150
	70CE2	70CD2	70CZ	30.070
	70CE2	70CD2	70CB	151.47
	70CE2	70CD2	70CE1	59.810
	70CE2	70CD2	700Н	19.220
10	70CE2	70CD2	70CA	143.09
	70CG	70CD2	70CD1	30.960
	70CG	70CD2	70CZ	91.040
	70CG	70CD2	70CB	31.150
	70CG	70CD2	70CE1	61.300
15	· 70CG	70CD2	700Н	101.91
	70CG	70CD2	70CA	23.850
	70CD1	70CD2	70CZ	60.090
	70CD1	70CD2	70CB	61.930
	70CD1	70CD2	70CE1	30.340
20	70CD1	70CD2	700Н	70.980
	70CD1	70CD2	70CA	53.880
	70CZ	70CD2	70CB	121.70
,	. 70CZ	70CD2	70CE1	29.750
	70CZ	70CD2	700H	10.950
25	70CZ	70CD2	70CA	113.46
	70CB	70CD2	70CE1	92.130
	70CB	70CD2	, 700Н	132.34
	70CB	70CD2	70CA	15.060
	70CE1	70CD2	700H	40.660
30	70CE1	70CD2	70CA	83.920
	700Н	70CD2	70CA	124.41
	70CD2	70CE2	70CZ	119.98
	70CD2	70CE2	700H	149.77
	70CD2	70CE2	70CE1	90.330
35	70CD2	70CE2	70CG	29.590
	70CD2	70CE2	70CD1	59.850
	70CD2	70CE2	70CB	18.490
	70CZ	70CE2	700Н	29.900
	70CZ	70CE2	70CE1	29.650
40	70CZ	70CE2	70CG	90.400
	70CZ	70CE2	70CD1	60.140
	70CZ	70CE2	70CB	101.79
	700Н	70CE2	70CE1	59.530
	•			478

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	700H	70CE2	70CG	120.21
	700н	70CE2	70CD1	89.990
	700н	70CE2	70CB	131.38
	70CE1	70CE2	70CG	60.750
5	70CE1	70CE2	70CD1	30.480
	70CE1	70CE2	70CB	72.220
	70CG	70CE2	70CD1	30.260
	70CG	70CE2	70CB	11.880
	70CD1	70CE2	70CB	41.820
10	700Н	70CZ	70CE1	119.71
	700Н	70CZ	70CE2	119.76
	700н	70CZ	70CD1	150.31
	700Н	70CZ	70CD2	149.60
	700H	70CZ	70CG	176.52
15	70CE1	70CZ	70CE2	120.47
	70CE1	70CZ	70CD1	30.730
	70CE1	70CZ	70CD2	90.520
•	70CE1	70CZ	70CG	60.620
	70CE2	70CZ	70CD1	89.750
20	70CE2	70CZ	70CD2	29.950
	70CE2	70CZ	70CG	59.860
	70CD1	70CZ	70CD2	59.800
	70CD1	70CZ	70CG	29.890
•	70CD2 `	70CZ	70CG	29.910
25	70CZ	7,00Н	70CE1	30.260
	70CZ	700Н	70CE2	30.340
	70CZ	700H	70CD2	19.450
	70CZ	700Н	70CD1	18.980
	70CE1	700Н	70CE2	60.580
30	70CE1	700н	70CD2	49.620
	70CE1	700н	70CD1	11.390
	70CE2	700н	70CD2	11.010
	70CE2	700H	70CD1	49.240
	70CD2	700H	70CD1	38.260
35	700	70C	71N	123.14
	700	70C	70CA	120.09
	700	70C	71CA	92.570
	700	70C	70N	99.070
	700	70C	70CB	99.330
40	700	70C	71C	78.860
	700	70C	70CG	105.60
	700	70C	72N	56.760
	700	70C	70CD1	125.74
				479

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	700	70C	71CB	108.48
	700	70C	, 710	90.870
	700	70C	27CE	75.140
	71N	70C	70CA	116.77
5	71N	70C	71CA	30.570
	71N	70C	. 70N	130.09
	71N	70C	70CB	128.41
	71N	70C	71C	50.660
	71N	70C	70CG	105.64
10	71N	70C	72N	71.070
	71N	70C	70CD1	85.130
	71N	70C	71CB	15,220
	71N	70C	710	47.160
	71N	70C	27CE	81.520
15	70CA	70C	71CA	147.33
	70CA	70C	70N	33.980
	70CA	70C	70CB	34.980
	70CA	70C	71C	149.00
	70CA	70C	70CG	55.070
20	70CA	70C	72N	156.37
	. 70CA	70C	70CD1	57.190
	70CA	70C	71CB	131.27
	70CA	70C	710	132.91
	70CA	70C	27CE	115.72
25	71CA	70C	70N	149.80
	71CA .	70C	70CB	147.07
	71CA	70C	71C	29.080
	71CA	70C	70CG	118.97
	71CA	70C	72N	43.930
30	71CA	70C	70CD1	104.65
	71CA	70C	71CB	16.560
	71CA	70C	710	36.650
	71CA	70C	27CE	70.660
	70N	70C	70CB	57.950
35	· 70N	70C	71C	177.02
	70N	70C	70CG	84.620
	70N	70C	72N	155.82
	70N	70C	70CD1	90.970
	70N	70C	71CB	137.64
40	70N	70C	710	166.83
	70N	70C	27CE	85.480
	70CB	70C	71C	124.36
	70CB	70C	70CG	28.140
	•			480

WO 03/048733	PCT/US02/38715
W O 03/046/33	1 C1/0302/30/13

	70CB	70C	72N	121.93
	70CB	70C	70CD1	44.210
	70CB	70C	71CB	142.05
	70CB	70C	710	112.09
5	70CB	70C	27CE	142.09
	71C	70C	70CG	97.990
	71C	70C	72N	22.120
	71C	70C	70CD1	91.980
	71C	70C	71CB	42.180
10	71C	70C	710	16.150
•	71C	70C	27CE	91.900
	70CG	70C	72N	101.82
	70CG	70C	70CD1	22.380
	70CG	70C	71CB	116.61
15	70CG	70C	710	84.400
	70CG	70C	27CE	170.06
	72N	70C	70CD1	103.85
	72N	70C	71CB	59.890
	72N	70C	710	35.310
20	72N	70C	27CE	86.930
	70CD1	70C	71CB	97.910
	70CD1	70C	710	76.150
	70CD1	70C	27CE	159.11
,	71CB	70C	710	44.150
25	71CB	70C	27CE	71.800
,	710	70C	27CE	105.54
	70C	700	71N	29.440
	70C	700	70CA	33.310
	70C	700	71CA	61.030
30	70C	700	70N	56.030
	70C	700	70CB	56.220
	70C	700	72N	103.35
	70C	700	71C	78.330
	70C	700	27N	162.85
35	70C	700	70CG	55.410
	70C	700	27CE	86.530
	70C	700	27CB	134.75
	70C	700	27CA	157.10
	71N	700	70CA	62.750
40	71N	700	71CA	31.590
	71N	700	70N	82.720
	71N	700	70CB	82.340
	71N	700	72N	77.000
				481

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	WC	D 03/048733				PCT/US02/38715
		71N	700	71C	52.450	
+		71N	700	27N	157.23	
		71N	700	70CG	73.420	
		71N	700	27CE	76.870	
	5	71N	700	27CB	118.58	
•		7 ['] 1N	700	27CA	137.77	
		70CA	700	71CA	94.340	
		70CA	700	70N	29.900	
		70CA	700	70CB	30.770	
	10	70CA	700	72N	131.80	
		70CA	700	71C	108.22	
		70CA	700	27N	134.37	
		70CA	700	70CG	44.610	
		70CA	700	27CE	98.600	
	15	70CA	700	27CB	137.96	
		70CA	700	27CA	147.24	
	•	71CA	700	70N	111.73	
		71CA	700	70CB	110.81	•
		71CA	700	72N	49.690	
	20	71CA	700	71C	29.600	
	20	71CA	700	27N	128.54	
		71CA	700	70CG	95.550	
		71CA	700	27CE	.70.170	
	•	71CA	700	27CB	95.820	\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \
•	25	71CA	700	27CB 27CA	109.66	
	45	71CA 70N	700	70CB	48.090	
		70N 70N	700	70CB 72N	159.36	
		70N 70N	700	72N 71C	134.32	
		70N 70N	700	71C 27N	108.05	
	30		700	70CG	69.260	
	30	70N				
•		70N	700 700	27CE	82.110	
		70N	700	27CB	109.82	
		70N	700	27CA	117.61	
	25	70CB	700	72N	124.02	
	35	70CB	700	71C	109.62	
		70CB	700	27N	119.93	
		70CB	700	70CG	23.200	
		70CB	700	27CE	128.06	
	40	70CB	700	27CB	149.98	
	40	70CB	700	27CA	139.34	
		72N	700	71C	25.040	
		72N	700	27N	92.310	•
		72N	700	70CG	100.85	
					482	

WO 03/048733	PCT/US02/38715

	72N	700	27CE	96.810
	72N	700	27CB	83.640
	72N	700	27CA	80.850
	71C	700	27N	116.95
5	71C	700	70CG	87.670
	71C	700	27CE	94.180
	71C	700	27CB	100.37
	71C	. 700	27CA	103.44
	27N	700	70CG	128.88
10	27N	700	27CE	84.660
	27N	700	27CB	39.280
	27N	700	27CA	19.550
	70CG	700	27CE	140.73
	70CG	700	27CB	167.97
15	70CG	700	27CA	146.72
	27CE	700	. 27CB	48.260
	27CE	700	27CA	70.590
	27CB	700	27CA	22.440
	70C	71N	71CA	122.07
20	70C	71N	700	27.430
	70C	71N	70CA	34.070
	70C	71N	71CB	156.58
	70C	71N	71C	105.29
	70C	71N	710	114.85
25	70C	71N	72N	87.060
	70C	71N	70N	32.830
	70C	71N	, 70CB	34.210
	70C	71N	70CG	54.320
	70C	71N	70CD1	74.260
30	70C	71N	27CE	79.190
	71CA	71N	700	94.650
	71CA	71N	70CA	156.14
	71CA	71N	71CB	35.960
	71CA	71N	71C	34.730
35	71CA	71N	710	47.910
	71CA	, 71N	72N	41.570
	71CA	71N	70N	144.29
	71CA	71N	70CB	143.42
	71CA	71N	70CG	
40	71CA	71N	70CD1	131.98
	71CA	71N	27CE	76.210
	700	71N	70CA	61.500
	700	71N	71CB	129.74
				483

WO 03/048733	PCT/US02/38715
WO 03/048733	PCT/US02/3871:

	700	71N	71C	82.170
	700	71N	710	97.500
	700	71N	72N	62.170
	700	71N	70N	56.830
5	700	71N	70CB	57.590
	700	71N	70CG	71.060
	700	71N	70CD1	92.580
	700	71N	27CE	69.480
	70CA	71N	71CB	166.85
10	70CA	71N	71C	131.75
	70CA	71N	710	129.72
	70CA	71N	72N	117.88
	70CA	71N	70N	20.640
	70CA	71N	70CB	21.890
15	· 70CA	71N	70CG	43.780
	70CA	71N	70CD1	54.810
	70CA	71N	27CE	94.230
	71CB	71N	71C	60.910
	71CB	71N	710	59.960
20	71CB	71N	72N	75.260
	71CB	71N	70N	153.78
	71CB	71N	70CB	164.62
	71CB	71N	. 70CG.	1,40.81
	71CB	71N	70CD1	124.74
25 ·	71CB	71N	27CE	85.200
	71C	71N	710	21.860
	71C	71N	72N	20.690
	71C	71N	70N	138.03
	71C	71N	70CB	111.76
30	71C	71N	70CG	96.900
	71C	71N	70CD1	100.26
	71C	71N	27CE	101.90
	710	71N	72N	40.850
	710	71N	70N	145.40
35	710	71N	70CB	107.84
	710	71N	70CG	87.250
	710	71N	70CD1	84.080
	710	71N	27CE	122.09
	72N	71N	70N	118.89
40	72N	71N	- 70CB	101.86
	72N	71N	70CG	94.280
	72N	71N	70CD1	104.97
	72N	71N	27CE	89.110
•	•			484

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70N 71N 70CB 40.420 70N 71N 70CB 63.740 70N 71N 70CD1 75.300 70N 71N 70CD1 75.300 70N 71N 70CD 73.750 5 70CB 71N 70CD1 40.740 70CB 71N 70CD1 40.740 70CB 71N 70CD1 21.520 70CB 71N 70CD1 21.520 70CG 71N 70CD 13.04 10 70CD1 71N 27CE 133.04 10 70CD1 71N 71CA 71C 109.56 71N 71CA 71C 112.75 71N 71CA 71C 105.38 71N 71CA 71C 105.38 71N 71CA 70C 27.360 15 71N 71CA 70C 353.760 71N 71CA 70CA 14.920 71N 71CA 70CA 14.920 71N 71CA 70CA 15.46 71N 71CA 71C 109.60 71CB 71CA 71C 109.60 71CB 71CA 71C 109.60 71CB 71CA 71C 109.60 71CB 71CA 70C 160.54 25 71CB 71CA 70CA 124.20 71CB 71CA 70CA 124.20 71CB 71CA 70CA 124.20 71CB 71CA 70CA 123.62 71CB 71CA 70CA 123.62 71CB 71CA 70CA 123.62 71C 71CA 70CA 106.58 71C 71CA 70CA 106.32 71C 71CA 70CA 106.32 71C 71CA 70CA 106.32 71C 71CA 70CA 106.32 71C 71CA 70CA 106.14 71CA 70CA 106.14 71CA 70CA 106.14 71CA 70CA 106.14						
70N 71N 70CD1 75.300 70N 71N 27CE 73.750 5 70CB 71N 70CD 23.840 70CB 71N 70CD1 40.740 70CG 71N 27CE 109.99 70CG 71N 27CE 133.04 10 70CD1 71N 27CE 149.03 71N 71CA 71C 112.75 71N 71CA 71C 112.75 71N 71CA 71C 115.21 71N 71CA 71C 115.21 71N 71CA 70C 27.360 15 71N 71CA 70CA 14.920 71N 71CA 70CA		70N	1:71N	70CB	40.420	
5 70N 71N 27CE 73.750 5 70CB 71N 70CB 23.840 70CB 71N 27CE 109.99 70CG 71N 27CE 199.99 70CG 71N 27CE 133.04 10 70CD1 71N 27CE 149.03 71N 71CA 71CB 109.56 71N 71CA 71C 105.38 71N 71CA 70C 27.360 15 71N 71CA 70C 27.360 15 71N 71CA 70CA 14.920 71N 71CA 70CA 14.920 71N 71CA 70CA 149.20 71N 71CA 71CA 70CA 19.60		70N	71N	70CG	63.740	
5 70CB 71N 70CG 23.840 70CB 71N 70CD1 40.740 70CB 71N 27CE 109.99 70CG 71N 27CE 133.04 10 70CD1 71N 27CE 149.03 71N 71CA 71CB 109.56 71N 71CA 71C 112.75 71N 71CA 71C 127.58 71N 71CA 71C 125.38 71N 71CA 71C 125.38 71N 71CA 70C 15.38 71N 71CA 70C 15.36 71N 71CA 70C 35.760 71N 71CA 70CA 14.920 71N 71CA 70CA 14.920 71N 71CA 70CA 14.920 71N 71CA 70CA 14.920 71C 71CA 70CA 14.920 71CA 71CA 70C		70N	71N	70CD1	75.300	
70CB 71N 70CD1 40.740 70CB 71N 27CE 109.99 70CG 71N 70CD1 21.520 70CG 71N 70CD1 21.520 70CG 71N 27CE 133.04 10 70CD1 71N 27CE 149.03 71N 71CA 71CB 109.56 71N 71CA 71C 112.75 71N 71CA 71C 105.38 71N 71CA 70C 27.360 15 71N 71CA 70C 135.760 71N 71CA 70C 153.760 71N 71CA 70CA 14.920 71N 71CA 70CA 14.920 71N 71CA 70CA 115.46 71N 71CA 70C 136.21 71N 71CA 71C 109.60 71CB 71CA 71C 109.60 71CB 71CA 71C 109.60 71CB 71CA 70C 136.21 71CB 71CA 70C 136.21 71CB 71CA 70C 124.20 71CB 71CA 70C 160.54 25 71CB 71CA 70CA 124.20 71CB 71CA 70CA 124.20 71CB 71CA 70CA 124.20 71CB 71CA 70CA 129.262 71CB 71CA 70CA 129.262 71CB 71CA 70CA 100.93 71C 71CA 70CA 100.93 71C 71CA 70CA 106.58 71C 71CA 70CA 106.14 71CA 70CA 106.40 70C 71CA 70		70N	71N	27CE	73.750	
70CB 71N 27CE 109.99 70CG 71N 70CD1 21.520 70CG 71N 27CE 133.04 10 70CD1 71N 27CE 149.03 71N 71CA 71CB 109.56 71N 71CA 71C 112.75 71N 71CA 71C 105.38 71N 71CA 70C 27.360 15 71N 71CA 70C 33.760 71N 71CA 70C 115.21 71N 71CA 70C 33.760 71N 71CA 70CA 14.920 71N 71CA 70CA 14.920 71N 71CA 70CA 14.920 71N 71CA 70CA 16.960 71CB 71CA 71C 109.60 71CB 71CA 71C 109.60 71CB 71CA 70C 136.21 71CB 71CA 70C 136.21 71CB 71CA 70C 160.54 25 71CB 71CA 70C 124.20 26 71CB 71CA 70C 160.54 27 71CB 71CA 70C 101.06 30 71C 71CA 70CA 124.20 71C 71CA 70C 101.06 31 71C 71CA 70CA 106.58 71C 71CA 70CA 106.14 71CA 70CC 71CA 70CA 106.06 70C 71CA 70CA 106.40 70C 71	5	70CB	71N	70CG	23.840	
70CG 71N 70CD1 21.520 70CG 71N 27CE 133.04 10 70CD1 71N 27CE 133.04 71N 71CA 71CB 109.56 71N 71CA 71C 112.75 71N 71CA 71C 105.38 71N 71CA 70C 27.360 15 71N 71CA 70C 27.360 15 71N 71CA 70C 35.760 71N 71CA 70CA 14.920 71N 71CA 70CA 14.920 71N 71CA 70CA 14.920 71N 71CA 70CA 115.46 71N 71CA 70CA 115.46 71N 71CA 70CA 12.46 71N 71CA 70CA 12.47 71CB 71CA 71C 109.60 71CB 71CA 71C 109.60 71CB 71CA 70C 136.21 71CB 71CA 70C 136.21 71CB 71CA 70C 160.54 25 71CB 71CA 70CA 124.20 71CB 71CA 70CA 124.20 71CB 71CA 70CA 124.20 71CB 71CA 70C 101.06 30 71C 71CA 70C 101.06 30 71C 71CA 70C 87.880 71C 71CA 70C 87.880 71C 71CA 70CA 106.58 71C 71CA 70CA 106.58 71C 71CA 70CA 106.58 71C 71CA 70CA 106.58 71C 71CA 70CA 106.32 71C 71CA 70CA 106.14 71CA 70CA 106.40 70C 71CA 70CA 106.40		70CB	71N '	. 70CD1	40.740	
TOCG		70CB	71N	27CE	109.99	•
10		70CG	. 71N	70CD1	21.520	
71N 71CA 71CB 109.56 71N 71CA 71C 112.75 71N 71CA 71C 105.38 71N 71CA 70C 27.360 15 71N 71CA 70N 115.21 71N 71CA 700 53.760 71N 71CA 70CA 14.920 71N 71CA 70CA 14.920 71N 71CA 70CA 115.46 71N 71CA 70CA 115.46 71N 71CA 71CA 109.60 71CB 71CA 71C 109.60 71CB 71CA 70C 136.21 71CB 71CA 70C 136.21 71CB 71CA 70C 128.74 71CB 71CA 70C 128.74 71CB 71CA 70CA 124.20 71CB 71CA 70CA 124.20 71CB 71CA 70CA 124.20 71CB 71CA 70CA 124.20 71CB 71CA 70C 100.93 71C 71CA 70C 101.06 30 71C 71CA 70C 101.06 30 71C 71CA 70C 101.06 30 71C 71CA 70CA 106.58 71C 71CA 70CA 106.32 71C 71CA 70CA 106.32 71C 71CA 70CA 106.32 71C 71CA 70CA 106.32 71C 71CA 70CA 106.14 71CA 70CA 106.40 70C		70CG	71N	27CE	133.04	
71N 71CA 71C 112.75 71N 71CA 71O 105.38 71N 71CA 70C 27.360 15 71N 71CA 70C 27.360 16 71N 71CA 70C 53.760 71N 71CA 70CA 14.920 71N 71CA 70CA 14.920 71N 71CA 70CA 14.920 71N 71CA 70CA 15.46 71N 71CA 70CA 15.46 71N 71CA 70CA 16.99.910 71CB 71CA 71C 109.60 71CB 71CA 71C 136.21 71CB 71CA 70C 136.21 71CB 71CA 70CA 124.20 71CB 71CA 70CA 124.20 71CB 71CA 70CA 124.20 71CB 71CA 70CA 123.62 71CB 71CA 70CA 124.20 71CB 71CA 70CA 101.06 30 71C 71CA 70C 101.06 30 71C 71CA 70CA 106.58 71C 71CA 70CA 106.14 71CA 70CC 71CA 70CA 106.14 71CA 70CC 71CA 70CA 106.10 70C 71CA 70CA 12.450	10	70CD1	71N	27CE	149.03	· .
71N 71CA 71O 105.38 71N 71CA 70C 27.360 15 71N 71CA 70C 53.760 71N 71CA 70CA 14.920 71N 71CA 70CA 14.920 71N 71CA 70CA 14.920 71N 71CA 70CA 82.300 20 71CB 71CA 71C 109.60 71CB 71CA 71C 109.60 71CB 71CA 70C 136.21 71CB 71CA 70C 136.21 71CB 71CA 70C 160.54 25 71CB 71CA 70CA 124.20 71CB 71CA 70CA 124.20 71CB 71CA 70CA 124.20 71CB 71CA 70CA 126.36 71C 71CA 70C 101.06 30 71C 71CA 70C 101.06 30 71C 71CA 70C 101.06 30 71C 71CA 70CA 106.58 71C 71CA 70CA 106.14 71O 71CA 70CA 106.14		71N	71CA	71CB	109.56	
71N		71N	71CA	71C	112.75	
15		71N	71CA	710	105.38	
71N 71CA 70C 53.760 71N 71CA 70CA 14.920 71N 71CA 72CA 115.46 71N 71CA 27CE 82.300 20 71CB 71CA 71C 109.60 71CB 71CA 71C 89.910 71CB 71CA 70C 136.21 71CB 71CA 70C 160.54 25 71CB 71CA 70CA 124.20 71CB 71CA 70CA 124.20 71CB 71CA 70CA 124.20 71CB 71CA 70CA 124.20 71CB 71CA 70C 101.06 30 71C 71CA 70C 101.06 30 71C 71CA 70C 101.06 30 71C 71CA 70C 101.06 31 71C 71CA 70C 103.70 71C 71CA 70CA 106.58 71C 71CA 70CA 106.14 71O 71CA 72CA 47.270 40 71C 71CA 72CA 12.450		71N	71CA	70C	27.360	
71N 71CA 70CA 14.920 71N 71CA 72CA 115.46 71N 71CA 27CE 82.300 20 71CB 71CA 71C 109.60 71CB 71CA 70C 136.21 71CB 71CA 70C 136.21 71CB 71CA 70C 160.54 25 71CB 71CA 70C 124.20 71CB 71CA 70C 124.20 71CB 71CA 70CA 124.20 71CB 71CA 70C 101.06 30 71C 71CA 70C 101.06 30 71C 71CA 70CA 106.58 71C 71CA 70CA 106.32 71C 71CA 70CA 106.32 71C 71CA 70CA 106.32 71C 71CA 70CA 106.14 71CA 70CC 71CA 72N 92.660 70C 71CA 72N 92.660 70C 71CA 70CA 12.450	15	71N	71CA	72N	115.21	
71N 71CA 72CA 115.46 71N 71CA 27CE 82.300 20 71CB 71CA 71C 109.60 71CB 71CA 71C 89.910 71CB 71CA 70C 136.21 71CB 71CA 70C 136.21 71CB 71CA 70C 160.54 25 71CB 71CA 70CA 124.20 71CB 71CA 70CA 124.20 71CB 71CA 70CA 123.62 71CB 71CA 70C 101.06 30 71C 71CA 70C 101.06 30 71C 71CA 70CA 106.58 71C 71CA 70CA 106.32 71C 71CA 70CA 106.32 71C 71CA 70CA 106.32 71C 71CA 70CA 106.14 71C 71CA 70CA 106.14 71C 71CA 70CA 106.14 71C 71CA 72CA 47.27C 40 71C 71CA 72CA 12.450		71N	71CA	700	53.760	
71N 71CA 27CE 82.300 71CB 71CA 71C 109.60 71CB 71CA 71O 89.910 71CB 71CA 70C 136.21 71CB 71CA 70O 160.54 25 71CB 71CA 70CA 124.20 71CB 71CA 72CA 123.62 71CB 71CA 72CA 123.62 71CB 71CA 70C 101.06 30 71C 71CA 70C 101.06 30 71C 71CA 70CA 106.58 71C 71CA 70CA 106.14 71C 71CA 70CA 106.14 71C 71CA 70CA 106.14 71C 71CA 72CA 20.91 40 71C 71CA 72CA 27CE 162.06 70C 71CA 72CA 12.450		.71N	71CA	70CA	14.920	
20		71N	·71CA	72CA	115.46	
71CB 71CA 71O 89.910 71CB 71CA 70C 136.21 71CB 71CA 72N 128.74 71CB 71CA 70O 160.54 25 71CB 71CA 70CA 124.20 71CB 71CA 72CA 123.62 71CB 71CA 71CA 71O 26.360 71C 71CA 71C 72CA 101.06 30 71C 71CA 70C 101.06 30 71C 71CA 70CA 106.58 71C 71CA 70CA 106.58 71C 71CA 70CA 106.58 71C 71CA 70CA 106.32 71C 71CA 70CA 106.32 710 71CA 70CA 106.14 710 71CA 70CA 106.14 710 71CA 72CA 47.270 40 710 71CA 72CA 106.14 710 71CA 72CA 106.40 70C 71CA 72N 92.660 70C 71CA 72N 92.660 70C 71CA 70O 26.400 70C 71CA 70CA 12.450		· 71N	71CA	27CE	82.300	
71CB 71CA 70C 136.21 71CB 71CA 72N 128.74 71CB 71CA 70O 160.54 25 71CB 71CA 70CA 124.20 71CB 71CA 72CA 123.62 71CB 71CA 71CA 710 26.360 71C 71CA 70C 101.06 30 71C 71CA 70C 101.06 30 71C 71CA 70C 20.88 71C 71CA 70C 101.06 31 71C 71CA 70C 106.58 71C 71CA 70CA 106.58 71C 71CA 72CA 20.910 71C 71CA 72CA 20.910 71C 71CA 70CA 106.32 710 71CA 70CA 106.32 710 71CA 70CA 106.14 710 71CA 70CA 106.14 710 71CA 72CA 47.270 40 710 71CA 72CA 162.06 70C 71CA 70C 26.400 70C 71CA 70C 26.400 70C 71CA 70C 26.400 70C 71CA 70C 26.400 70C 71CA 70CA 12.450	20	71CB	71CA	71C	109.60	•
71CB 71CA 72N 128.74 71CB 71CA 70O 160.54 25 71CB 71CA 70CA 124.20 71CB 71CA 72CA 123.62 71CB 71CA 71CA 27CE 102.93 71C 71CA 71CA 70C 101.06 30 71C 71CA 70C 101.06 30 71C 71CA 70CA 106.58 71C 71CA 70CA 106.58 71C 71CA 72CA 20.910 71C 71CA 72CA 20.910 71C 71CA 70CA 106.32 71C 71CA 70CA 106.32 71C 71CA 70CA 106.14 71C 71CA 70CA 106.14 71C 71CA 72CA 20.91C 71C 71CA 70CA 106.14 71C 71CA 72CA 106.14 71C 71CA 72CA 106.14 71C 71CA 72CA 106.14 71CA 71CA 72CA 106.40 70C 71CA 71CA 72CA 12.450		71CB	71CA	710	89.910	
71CB 71CA 700 160.54 25 71CB 71CA 70CA 124.20 71CB 71CA 72CA 123.62 71CB 71CA 27CE 102.93 71C 71CA 71CA 70C 101.06 30 71C 71CA 72N 29.260 71C 71CA 70CA 106.58 71C 71CA 70CA 106.58 71C 71CA 72CA 20.910 71C 71CA 70CA 106.32 71C 71CA 70CA 106.32 71C 71CA 70CA 106.14 71C 71CA 70CA 106.14 71C 71CA 72CA 47.27C 40 71C 71CA 72CA 27CE 162.06 70C 71CA 72CA 92.660 70C 71CA 72CA 92.660 70C 71CA 72CA 106.40 70C 71CA 72CA 12.450		71CB	71CA	70C	136.21	
25 71CB 71CA 70CA 124.20 71CB 71CA 72CA 123.62 71CB 71CA 27CE 102.93 71C 71CA 71O 26.360 71C 71CA 70C 101.06 30 71C 71CA 70C 101.06 30 71C 71CA 70CA 106.58 71C 71CA 70CA 106.58 71C 71CA 72CA 20.910 71C 71CA 70CA 106.32 71C 71CA 70CA 106.32 71O 71CA 70CA 106.32 71O 71CA 70CA 106.14 71O 71CA 70CA 106.14 71O 71CA 72CA 47.270 40 71C 71CA 72CA 162.06 70C 71CA 70C 26.400 70C 71CA 70CA 12.450		71CB	71CA	72N	128.74	
71CB 71CA 72CA 123.62 71CB 71CA 27CE 102.93 71C 71CA 710 26.360 71C 71CA 70C 101.06 30 71C 71CA 72N 29.260 71C 71CA 70CA 106.58 71C 71CA 70CA 106.58 71C 71CA 72CA 20.910 71C 71CA 70CA 106.32 71C 71CA 70CA 106.32 71O 71CA 72CA 72N 55.620 71O 71CA 70CA 106.14 71O 71CA 72CA 47.270 40 71C 71CA 72CA 106.14		71CB	71CA	700	160.54	Tallor Programmer Control of the Con
71CB 71CA 27CE 102.93 71C 71CA 71O 26.360 71C 71CA 70C 101.06 30 71C 71CA 72N 29.260 71C 71CA 70O 87.880 71C 71CA 70CA 106.58 71C 71CA 72CA 20.910 71C 71CA 27CE 135.72 35 710 71CA 70C 106.32 710 71CA 72N 55.620 710 71CA 70C 106.14 710 71CA 70CA 106.14 710 71CA 72CA 47.270 40 710 71CA 27CE 162.06 70C 71CA 72N 92.660 70C 71CA 70O 26.400 70C 71CA 70CA 12.450	25	71CB	71CA	70CA	124.20	
71C 71CA 71O 26.360 71C 71CA 70C 101.06 30 71C 71CA 72N 29.260 71C 71CA 70O 87.880 71C 71CA 70CA 106.58 71C 71CA 72CA 20.910 71C 71CA 72CA 20.910 71C 71CA 70C 106.32 710 71CA 72N 55.620 710 71CA 70O 103.70 710 71CA 70CA 106.14 710 71CA 72CA 47.270 40 71C 71CA 72N 92.660 70C 71CA 72N 92.660 70C 71CA 70O 26.400 70C 71CA 70CA 12.450		71CB	71CA	72CA	123.62	
71C 71CA 70C 101.06 71C 71CA 72N 29.260 71C 71CA 70O 87.880 71C 71CA 70CA 106.58 71C 71CA 72CA 20.910 71C 71CA 27CE 135.72 35 710 71CA 70C 106.32 710 71CA 72N 55.620 710 71CA 70CA 106.14 710 71CA 72CA 47.270 40 71C 71CA 27CE 162.06 70C 71CA 70CA 12.450		71CB	71CA	27CE	102.93	
30 71C 71CA 72N 29.260 71C 71CA 70O 87.880 71C 71CA 70CA 106.58 71C 71CA 72CA 20.910 71C 71CA 72CE 135.72 35 710 71CA 70C 106.32 710 71CA 72N 55.620 710 71CA 70O 103.70 710 71CA 70CA 106.14 710 71CA 72CA 47.270 40 710 71CA 72CE 162.06 70C 71CA 70O 26.400 70C 71CA 70CA 12.450		71C	71CA	710	26.360	
71C 71CA 70O 87.880 71C 71CA 70CA 106.58 71C 71CA 72CA 20.910 71C 71CA 72CE 135.72 35 710 71CA 70C 106.32 710 71CA 72N 55.620 710 71CA 70O 103.70 710 71CA 70CA 106.14 710 71CA 72CA 47.270 40 71C 71CA 72CA 47.270 40 71C 71CA 72CA 47.270 70C 71CA 70O 26.400 70C 71CA 70O 26.400 70C 71CA 70CA 12.450		71C	71CA	70C	101.06	
71C 71CA 70CA 106.58 71C 71CA 72CA 20.910 71C 71CA 27CE 135.72 35 710 71CA 70C 106.32 710 71CA 72N 55.620 710 71CA 70O 103.70 710 71CA 70CA 106.14 710 71CA 72CA 47.270 40 710 71CA 27CE 162.06 70C 71CA 70O 26.400 70C 71CA 70CA 12.450	30	71C	71CA	72N	29.260	
71C 71CA 72CA 20.910 71C 71CA 27CE 135.72 35 710 71CA 70C 106.32 710 71CA 72N 55.620 710 71CA 70O 103.70 710 71CA 70CA 106.14 710 71CA 72CA 47.270 40 710 71CA 27CE 162.06 70C 71CA 70O 26.400 70C 71CA 70CA 12.450		71C	71CA	700	87.880	
71C 71CA 27CE 135.72 710 71CA 70C 106.32 710 71CA 72N 55.620 710 71CA 70O 103.70 710 71CA 70CA 106.14 710 71CA 72CA 47.270 40 710 71CA 27CE 162.06 70C 71CA 72N 92.660 70C 71CA 70O 26.400 70C 71CA 70CA 12.450		71C	71CA	70CA	106.58	٠.
35 710 71CA 70C 106.32 710 71CA 72N 55.620 710 71CA 70O 103.70 710 71CA 70CA 106.14 710 71CA 72CA 47.270 40 710 71CA 27CE 162.06 70C 71CA 72N 92.660 70C 71CA 70O 26.400 70C 71CA 70CA 12.450		71C	71CA	72CA	20.910	
710 71CA 72N 55.620 710 71CA 700 103.70 710 71CA 70CA 106.14 710 71CA 72CA 47.270 40 710 71CA 27CE 162.06 70C 71CA 72N 92.660 70C 71CA 70O 26.400 70C 71CA 70CA 12.450		71C	71CA	27CE	135.72	
710 71CA 700 103.70 710 71CA 70CA 106.14 710 71CA 72CA 47.270 40 710 71CA 27CE 162.06 70C 71CA 72N 92.660 70C 71CA 700 26.400 70C 71CA 70CA 12.450	35	710	71CA	70C	106.32	
710 71CA 70CA 106.14 710 71CA 72CA 47.270 40 710 71CA 27CE 162.06 70C 71CA 72N 92.660 70C 71CA 70O 26.400 70C 71CA 70CA 12.450		710	71CA	72N	55.620	
710 71CA 72CA 47.270 710 71CA 27CE 162.06 70C 71CA 72N 92.660 70C 71CA 70O 26.400 70C 71CA 70CA 12.450		710	71CA	700	103.70	
40 710 71CA 27CE 162.06 70C 71CA 72N 92.660 70C 71CA 70O 26.400 70C 71CA 70CA 12.450		710	71CA	70CA	106.14	
70C 71CA 72N 92.660 70C 71CA 70O 26.400 70C 71CA 70CA 12.450		710	71CA	72CA	47.270	
70C 71CA 70O 26.400 70C 71CA 70CA 12.450	40	710	71CA	27CE	162.06	
70C 71CA 70CA 12.450		70C	71CA	72N	92.660	
		70C	71CA	700	26.400	
485		70C	71CA	70CA	12.450	
				•	485	

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•	70C	71CA	72CA	95.460
	70C	71CA	.27CE	72.980
	72N	71CA	700	70.710
	72N	71CA	70CA	102.91
5	72N	71CA	72CA	8.350
	72N	71CA ·	27CE	106.47
	700	71CA	70CA	38.850
•	700	71CA	72CA	75.600
	700	71CA	27CE	67.380
10	70CA	71CA	72CA	104.61
	70CA	71CA	27CE	77.110
	72CA	71CA	27CE	114.81
	71CA	71CB	71N	34.470
	71CA	71CB	71C	35.620
15	71CA	71ÇB	710	57.930
	71CA	71CB	72N	32.120
	71CA	71CB	70C	27.230
	71N	71CB	71C	61.000
	71N	71CB	710	72.360
20	71N	71CB	72N	64.020
	71N	71CB	70C	8.190
	71C	71CB	710	25.670
	71C "	71CB	, · · 72N · ·	14.610
	71C	71CB	70C	56.950
25	710	71CB	72N	39.060
	710	71CB	70C	71.620
	72N	71CB	70C	58.090
	710	71C	72N	123.77
	710	71C	71CA	119.82
30	710	71C	72CA	93.990
	710	71C	71CB	92.930
	710	71C	71N	109.08
	710	71C	70C	119.12
	710	71C	700	134.27
35	710	71C	72CB	88.520
	72N	71C	71CA	116.41
	72N	71C	72CA	29.780
	72N	71C	71CB	137.30
	72N	71C	71N	118.01
40	72N	71C	70C	96.550
	72N	71C	700	73.760
	72N	71C	72CB	43.410
	71CA	71C	72CA	146.18
	•			486

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	71CA	71C	71CB	34.780
	71CA	71C	71N	32.530
	71CA	71C	70C	49.860
	71CA	71C	700	62.520
5	71CA	71C	72CB	141.88
	72CA	71C	71CB	155.41
	72CA	71C	71N	139.72
	72CA	71C	70C	115.69
	72CA	71C	700	94.990
10	72CA	71C	72CB	27.030
	71CB	71C	71N	58.090
	71CB	71C	70C	80.870
	71CB	71C	700	96.960
	71CB	71C	72CB	129.92
15	71 N ,	71C	70C	24.050
	71N	71C	700	45.370
	71N	71C	72CB	161.09
	70C	71C	700	22.810
	70C	71C	72CB	139.51
20	700	71C	72CB	116.94
	71C	710	72N	29.380
	71C	710	71CA	33.810
	71C	710	72CA	60.310
	71C ·	710	71CB	61.410
25 .	71C	710	71N	49.060
	71C	710	72CB	70.480
	71C	710	70C	44.730
	72N	710	71CA	63.190
	72N	710	72CA	30.930
30	72N	710	71CB	88.790
	72N	710	71N	74.700
	72N	710	72CB	45.310
	72N	710	70C	64.140
	71CA	710	72CA	94.120
35	71CA	710	71CB	32.160
	71CA	710	71N	26.700
	71CA	710	72CB	100.98
	71CA	710	70C	37.030
	72CA	710	71CB	117.50
40	72CA	710	71N	102.84
	72CA	710	72CB	26.060
	72CA	710	70C	88.620
	71CB	710	71N	47.680
				107

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	71CB	710	72CB	111.77
	71CB	710	70C	64.230
	71N	710	72CB	119.19
	71N	710	70C	17.990
5	72CB	710	70C	109.31
	71C	72N	72CA	123.26
	71C	72N	710	26.850
	71C	72N	72CB	114.53
	71C	72N	71CA	34.330
10	71C	72N	700	81.190
	71C	72N	270	146.86
	71C	72N	71N	41.300
	71C	72N	70C	61.330
	71C	72N	71CB	28.090
15	· 71C ·	72N	72CG	120.73
	72CA	72N	710	96.410
•	72CA	72N	72CB	36.130
	72CA	72N	71CA	157.59
	72CA	72N	700	130.94
20	72CA	72N	270	87.240
	72CA	72N	71N	149.24
	72CA	72N	70C	139.50
	72CA	72N	71CB	143.24
	72CA	72N	72CG	24.380
25	710	72N	72CB	93.520
	710	72N	71CA	61.190
	710	72N	700	99.610
	710	72N	270	166.12
	710	72N	71N	64.450
30	710	72N	70C	80.560
	710	72N	71CB	52.140
	. 710	72N	72CG	96.790
	72CB	72N	71CA	136.83
	72CB	72N	700	163.29
35	72CB	72N	270	81.510
	72CB	72N	71N	155.58
	72CB	72N	70C	172.50
	72CB	72N	71CB	117.74
	72CB	72N	72CG	12.020
40	71CA	72N	700	59.600
	71CA	72N	270	114.35
	71CA	72N	71N	23.230
	71CA	72N	70C	43.410
	•			488

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•	71CA	72N	71CB	19.140
	71CA	72N	72CG	147.56
	700	72N	270	87.890
	700	72N	71N ·	40.840
5	700 ,	72N	70C	19.890
	700	72N	71CB	78.740
	700	72N	72CG	152.63
	270	72N	71N	117.30
	270	72N	70C	105.29
10	270	72N	71CB	119.05
	270	72N	72CG	81.040
	71N	72N	70C	21.880
	71N	72N	71CB	40.720
	71N	72N	72CG	161.22
15	70C	72N	71CB	62.020
	70C	72N	72CG	163.70
	71CB	72N	72CG	128.46
	72N	72CA	72CB	109.52
	72N	72CA	71C	26.960
20	72N	72CA	72CG	141.87
	72N	72CA	710	52.660
	72N	72CA	72CD2	146.65
	72N'	72CA	72CD1	139.86
	72N	72CA	270	68.520
25	. 72N	72CA	71CA	14.060
	72CB	72CA	71C	105.89
	72CB	72CA	72CG	32.600
	72CB	72CA	710	99.550
	72CB	72CA	72CD2	44.050
30	72CB	72CA	72CD1	43.570
	72CB	72CA	270	87.730
	72CB	72CA	71CA	107.84
	71C	72CA	72CG	135.26
	71C	72CA	710	25.700
35	71C	72CA	72CD2	126.95
	71C	72CA	72CD1	148.66
	71C	72CA	270	94.770
	71C	72CA	71CA	12.900
	72CG	72CA	710	119.79
40	72CG	72CA	72CD2	21.870
	72CG	72CA	72CD1	21.560
	72CG	72CA	270	97.590
	72CG	72CA	71CA	139.89
	•		•	489

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	710	72CA	72CD2	104.93
	710	72CA	72CD1	140.32
	710	72CA	270	119.83
	710	7.2CA	71CA	38.610
5	72CD2	72CA	72CD1	41.260
	72CD2	72CA	270	119.45
	72CD2	72CA	71CA	136.99
	72CD1	72CA	270	79.620
	72CD1	72CA	71CA	146.25
10	270	72CA	71CA	82.130
	72CG	72CB	72CA	114.08
	72CG	72CB	72N	148.14
	72CG	72CB	72CD2	28.400
	72CG	72CB	72CD1	28.260
15	72CG	72CB	71C	153.74
	72CG	72CB	710	137.43
	72CG	.72CB	72CE2	18.460
	72CG	72CB	72CE1	18.190
	72CG	72CB	270	114.19
20	72CA	72CB	72N	34.350
	72CA	72CB	72CD2	110.80
	72CA	72CB	72CD1	111.57
	72CA ··	72CB	71C	47.080
	72CA	72CB	710	54.380
25	72CA	72CB	72CE2	112,85
	72CA	72CB	72CE1	113.46
	72CA	72CB	270	68.670
	72N	72CB	72CD2	140.56
	72N	72CB	72CD1	136.51
30	72N	72CB	71C	22.060
	72N	72CB	710	41.170
	72N	72CB	72CE2	145.55
	72N	72CB	72CE1	142.65
	72N	72CB	270	59.200
35	72CD2	72CB	72CD1	56.660
	72CD2	72CB	71C	130.98
	72CD2	72CB	710	111.11
	72CD2	72CB	72CE2	9.950
	72CD2	72CB	72CE1	46.590
40 .	72CD2	72CB	270	141.36
	72CD1	72CB	71C	157.53
	72CD1	72CB	710	159.45
	72CD1	72CB	72CE2	46.710
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	72CD1	72CB	72CE1	10.080
	72CD1	72CB	270	86.740
	71C	72CB	710	20.990
•	71C	-72CB	72CE2	139.78
5	71C	72CB	72CE1	160.44
	71C	72CB	270	78.680
	710	72CB	72CE2	120.56
	710	72CB	72CE1	152.99
	710	72CB	270	99.520
10	72CE2	72CB	72CE1	36.640
•	72CE2	72CB	270	132.04
	72CE1	72CB	270	96.610
	72CD2	72CG	72CD1	118.70
	72CD2	72CG	72CB	120.48
15	72CD2	72CG	72CE2	29.700
	72CD2	72CG	72CE1	88.910
	72CD2	72CG	72CA	114.81
	72CD2	72CG	72CZ	59.270
	72CD2	72CG	72N	120.43
20	72CD1	72CG	72CB	120.81
	72CD1	72CG	72CE2	89.010
	72CD1	72CG	72CE1	29.800
	72CD1	72CG	72CA	115.91
*	72CD1	72CG	72CZ	59.430
25.	72CD1	72CG	72N	117.10
	72CB	72CG	72CE2	150.17
	72CB	72CG	72CE1	150.61
	72CB	72CG	72CA	33.320
	72CB	72CG	72CZ	179.28
30	72CB	72CG	72N	19.840
	72CE2	72CG	72CE1	59.210
	72CE2	72CG	72CA	136.56
	72CE2	72CG	72CZ	29.580
	72CE2	72CG	72N	146.64
35	72CE1	72CG	72CA	137.55
	72CE1	72CG	72CZ	29.630
	72CE1	72CG	72N	143.84
	72CA	72CG	72CZ	147.36
	72CA	72CG	72N	13.750
40	72CZ	72CG	72N	160.86
	72CG	72CD1	72CE1	120.63
	72CG	72CD1	72CD2	30.630
	72CG	72CD1	72CZ	90.830
				401

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	•			
72CG	72CD1	72CB	30.930	ŀ
72CG	72CD1	72CE2	60.910	ŀ
72CG	72CD1	280D1	142.39	ŀ
72CG	72CD1	28CG	124.62	
72CG	72CD1	72CA		ŀ
72CG	72CD1 -	280D2	•	ŀ
72CG	72CD1			ŀ
72CE1	·72CD1		·	ŀ
72CE1	•			ı
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			N. Carlotte and the control of the c	ŀ
	•		90.960	ŀ
		28CA	135.19	ŀ
72CB	72CD1	72CE2	91.840	ŀ
72CB	72CD1	280D1	136.58	
72CB	72CD1	-28CG	115.00	ŀ
72CB	72CD1	72CA	24.860	ı
72CB 72CB	72CD1 72CD1	72CA 28OD2	24.860 103.47	
			\cdot	
72CB	72CD1	280D2	103.47	
72CB - 72CB	72CD1 72CD1	280D2 28CA	103.47 95.310	
72CB · 72CB 72CE2	72CD1 72CD1 72CD1	280D2 28CA 280D1	103.47 95.310 108.17	
72CB 72CB 72CE2 72CE2	72CD1 72CD1 72CD1 72CD1	280D2 28CA 280D1 28CG	103.47 95.310 108.17 113.24	
72CB 72CB 72CE2 72CE2 72CE2	72CD1 72CD1 72CD1 72CD1 72CD1	280D2 28CA 280D1 28CG 72CA	103.47 95.310 108.17 113.24 96.530	
72CB 72CB 72CE2 72CE2 72CE2 72CE2	72CD1 72CD1 72CD1 72CD1 72CD1 72CD1	280D2 28CA 280D1 28CG 72CA 280D2	103.47 95.310 108.17 113.24 96.530 98.660	
72CB 72CB 72CE2 72CE2 72CE2 72CE2 72CE2	72CD1 72CD1 72CD1 72CD1 72CD1 72CD1 72CD1	280D2 28CA 280D1 28CG 72CA 280D2 28CA	103.47 95.310 108.17 113.24 96.530 98.660 152.31	
	72CG 72CG 72CG 72CG 72CG 72CG 72CG 72CE1 72CE1 72CE1 72CE1 72CE1 72CE1 72CE1 72CE1 72CE2 72CD2 72CZ 72CZ 72CZ 72CZ 72CZ 72CZ 72CZ 72C	72CG 72CD1 72CE1 72CD1 72CD2 72CD1 72CZ 72CD1	72CG 72CD1 72CE2 72CG 72CD1 28OD1 72CG 72CD1 28CG 72CG 72CD1 72CA 72CG 72CD1 28OD2 72CG 72CD1 28CA 72CE1 72CD1 72CD2 72CE1 72CD1 72CB 72CE1 72CD1 72CB 72CE1 72CD1 72CB 72CE1 72CD1 72CB 72CE1 72CD1 28OD1 72CE1 72CD1 28OD1 72CE1 72CD1 28OD2 72CE1 72CD1 72CA 72CE1 72CD1 72CA 72CD2 72CD1 72CB 72CD2 72CD1 72CB2 72CD2 72CD1 72CB2 72CD2 72CD1 72CA 72CD2 72CD1 72CA 72CD2 72CD1 72CB 72CD2 72CD1 72CB 72CD2	72CG 72CD1 72CE2 60.910 72CG 72CD1 28CD1 142.39 72CG 72CD1 28CG 124.62 72CG 72CD1 72CA 42.530 72CG 72CD1 28CA 122.27 72CE1 72CD1 72CD2 90.000 72CE1 72CD1 72CD2 29.800 72CE1 72CD1 72CB 151.55 72CE1 72CD1 72CB2 59.720 72CE1 72CD1 72CB 151.55 72CE1 72CD1 72CB 151.55 72CE1 72CD1 28CG 80.270 72CE1 72CD1 28CG 80.270 72CE1 72CD1 28CG 83.110 72CE1 72CD1 28CA 110.27 72CD2 72CD1 72CB 61.560 72CD2 72CD1 72CB 61.560 72CD2 72CD1 28CG 123.86 72CD2 72

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	280D1	72CD1	72CA	112.55
	280D1	72CD1	280D2	37.060
	280D1	72CD1	28CA	50.620
	28CG	72CD1	72CA	90.900
5	28CG	72CD1	280D2	20.050
	28CG	72CD1	28CA	40.080
	72CA	72CD1	280D2	78.630
	72CA	72CD1	28CA	79.860
	280D2	72CD1	28CA	53.660
10	72CG	72CD2	72CE2	120.82
	72CG	72CD2	72CD1	30.660
	72CG	72CD2	72CZ	91.020
	72CG	72CD2	72CB	31.120
	72CG	72CD2	72CE1	61.010
15	, 72CG	, 72CD2	72CA	43.310
	72CE2	72CD2	72CD1	90.160
*	72CE2	72CD2	72CZ	29.800
	72CE2	72CD2	72CB	151.94
	72CE2	72CD2	72CE1	59.810
20	72CE2	72CD2	72CA	147.84
	72CD1	72CD2	72CZ	60.360
	72CD1	72CD2	72CB	61.780
	72CD1	72CD2	72CE1	30.350
	72CD1	72CD2	72CA	69.800
25	72CZ	72CD2	72CB	122.14
	72CZ	72CD2	72CE1	30.010
	72CZ	72CD2	72CA	124.38
	72CB	72CD2	72CE1	92.130
	72CB	72CD2	72CA	25.150
30	72CE1	72CD2	72CA	97.470
	72CZ	72CE1	72CD1	120.06
	72CZ	72CE1	72CE2	30.110
	72CZ	72CE1	72CG	90.490
	72CZ	72CE1	280D1	128.03
35	72CZ	72CE1	72CD2	60.410
	72CZ	72CE1	28CG	126.46
	72CZ	72CE1	280D2	109.52
	72CZ	72CE1	72CB	101.69
	72CD1	72CE1	72CE2	89.950
40	72CD1	72CE1	72CG	29.570
	72CD1	72CE1	280D1	91.000
	72CD1	72CE1	72CD2	59.650
	72CD1	72CE1	28CG	75.900
				100

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	72CD1	72CE1	28OD2	75.000
	72CD1	72CE1	72CB	18.370
	72CE2	72CE1	72CG	60.390
	72CE2	72CE1	280D1	136,.30
5	72CE2	72CE1	72CD2	30.310
	72CE2	72CE1	28CG	123.13
	72CE2	72CE1	28OD2	103.74
	72CE2	72CE1	72CB	71.590
	72CG	72CE1	28OD1	111.96
10	72CG	72CE1	72CD2	30.080
	72CG	72CE1	28CG	93.450
	72CG	72CE1	280D2	83.970
	72CG	72CE1	72CB	11.210
	280D1	72CE1	72CD2	129.34
15	280D1	72CE1	28CG	19.220
	280D1	72CE1	28OD2	35.520
	280D1	72CE1	72CB	104.46
	72CD2	72CE1	28CG	110.49
	72CD2	72CE1	280D2	94.360
20	72CD2	72CE1	72CB	41.280
	28CG	72CE1	28OD2	19.440
	28CG	72CE1	72CB	86.970
	280D2	72CE1	72CB	.80.590
	72CZ	72CE2	72CD2	120.05
25	72CZ	72CE2	72CE1	30.170
	72CZ	72CE2	72CG	90.570
	72CZ	72CE2	72CD1	60.490
	72CZ	72CE2	72CB	101.94
	72CD2	72CE2	72CE1	89.890
30	72CD2	72CE2	72CG	29.480
	72CD2	72CE2	72CD1	59.560
	72CD2	72CE2	72CB	18.120
	72CE1	72CE2	72CG	60.400
	72CE1	72CE2	72CD1	30.320
35	72CE1	72CE2	72CB	71.770
	72CG	72CE2	72CD1	30.080
	72CG	72CE2	72CB	11.370
	72CD1	72CE2	72CB	41.450
	72CE2	72CZ	72CE1	119.73
40	72CE2	72CZ	72CD2	. 30.150
	72CE2	72CZ	72CD1	89.590
	72CE2	72CZ	72CG	59.850
	72CE2	72CZ	280D1	130.21
				494

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720	CE1	72CZ	72CD2	89.580	
720	CE1	72CZ	72CD1	30.140	•

	72CE1	12CZ	72CD2	89.580
	72CE1	72CZ	72CD1	30.140
	72CE1	72CZ	172CG	59.870
	72CE1	72CZ	280D1	34.880
5	72CD2	72CZ	72CD1	59.440
	72CD2	72CZ	72CG	29.700
	72CD2	72CZ	280D1	105.62
	72CD1	72CZ	72CG	29.740
	72CD1	72CZ	280D1	55.110
10	72CG	72CZ	280D1	80.010

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Table IIIB
Interatomic angle between residues in the active site of UPPS in complex with FPP

	AAIRII I F. I			
5	ATOM1	ATOM2	EMOTA .	ANGLE, degree
	79NH1	1C1	7.9NH2	36.680
	300D1	1C2	45NE2	73.500
	300D1	1C2	79NH1	123.81
	45NE2	1C2,	79NH1	54.230
10	710	1C4	71C	16.510
	710	1C5 ´	45CD2	138.38
	300D1	1C6	710	158.04
	49N	1C10	450	54.930
	49N	1C10	48C	22.570
15	49N	1C10	48CA	41.710
	49N	1C10	300D1	112.37
	49N	1C10	49CA	20.490
	450	1C10	48C	66.450
	450	1C10	48CA	60.290
20	450	1C10	300D1	80.140
	450	1C10	49CA	66.810
	48C	1C10	48CA	24.950
	48C	1C10	300D1	98.690
	48C	1C10	49CA	38.030
25	48CA	1C10	300D1	73.850
	48CA	1C10	49CA	60.970
	300D1	1C10	49CA	132.86
	143CE2	1C14	143CZ	22.460
	143CE2	1C14	143CD2	20.550
30	143CE2	1C14	91CG	154.92
	143CE2	1C14	91CA	166.15
	143CZ	1C14	143CD2	36.950
	143CZ	1C14	91CG	161.83
	143CZ	1C14	91CA	143.89
35	143CD2	1C14	91CG	134.76
	143CD2	1C14	91CA	159.08
	91CG	1C14	91CA	34.360
	49SD	1C15	94CG	72.370
	49SD	1C15	94CB	63.260
40	49SD	1C15	94CD1	62.610
	49SD	1C15	49CG	28.760
	49SD	1C15	900	60.290

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	94CG	1C15	94CB	23.960
	94CG	1C15	94CD1	22.200
	94CG	1C15	49CG	80.380
٠	94CG	1C15	900	71.370
5	94CB	1C15	94CD1	40.410
	94CB	1C15	49CG	81.980
	94CB	1C15	900	47.420
	94CD1	1C15	49CG	61.840
	94CD1	1C15	900	84.480
10	49CG	1C15	900	89.040
	79NH2	101A	45CE1	104.86
	79NH2	101A	79NH1	36.270
	79NH2	101A	31N	161.20
	45CE1	101A	79NH1	69.380
15	45CE1	101A	31N	73.460
	79NH1	101A	31N	141.07
	79NH2	102A	280D2	143.61
	29N	103A	30N	51.620
	29N	103A	31N	98.770
20	29N	103A	29C	42.330
	29N	103A	30CB	88.140
	29N	103A	29CA	21.740
	. 29N	103A	30CA	72.890
,	30N	103A	31N	53.440
25	30N	103A	29C	21.050
	30N	103A	30CB	40.610
	30N	103A	29CA	39.740
	30N	103A	30CA	21.320
	31N	103A	29C	56.440
30	31N	103A	30CB	47.440
	31N	103A	29CA	78.530
	31N	103A	30CA	38.230
	29C	103A	30CB	60.250
	29C	103A	29CA	23.500
35	29C	103A	30CA	37.980
	30CB	103A	29CA	80.270
	30CB	103A	30CA	23.300

103A

1PB

1PB

1PB

1PB

1PB

29CA

29N

29N

29N

29N

29CA

40

497

59.960

22.630

39.230 43.180

87.600

22.740

30CA

29CA

29C

30N

31N

29C

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	29CA	1PB	30N	36.770
	29CA	1PB	31N	73.860
	29C	1PB	30N	19.570
	29C	1PB	31N	51.200
5	30N	1PB	31N	45.170
	280 <u>D</u> 2	101B	29N	84.890
	280D2	101B	28CG	16.680
	29N	101B	28CG	68.950
	29CA	103B	32N	96.470
10	29CA	103B	32CB	86.020
	29CA	103B	29C	28.020
	29CA	103B	29N	26.430
	29CA	103B	290	41.610
	29CA	103B	30N	40.840
15	29CA	103B	31N	86.120
	29CA	103B	32CA	93.510
	32N	103B	32CB	45.930
	32N	103B	29C	74.560
	32N	103B	29N	119.84
20	32N	103B	290	55.800
	32N	103B	30N	80.770
	32N	103B	31N	48.860
	32N	103B	. 32CA	22.120
	32CB	103B	29C	83.310
25	32CB	103B	29N	111.02
	32CB	103B	290	65.280
	32CB	103B	30N	101.43
	32CB	103B	31N	92.340
	32CB	· 103B	32CA	23.970
30	29C	103B	29N	45.490
	29C	103B	290	20.200
	29C	103B	30N	20.670
	29C	103B	31N	58.520
	29C	103B	32CA	79.800
35	29N	103B	290	64.150
	29N	103B	30N	45.760
	29N	103B	31N	93.530
	29N	103B	32CA	119.86
	290	103B	30N	36.150
40	290	103B	31N	
	290	103B	32CA	59.600
	30N	103B	31N	48.360
	30N	103B	32CA	92.530
				408

31N 103B 32CA 70.170

Table IIIC
Interatomic angle between residues in the active site of UPPS in complex with IPP

5	with IPP			
	ATOM1	ATOM2	EMOTA	ANGLE, degree
	280D2	1C02	270	87.520
	280D2	1C02	28CB	36.210
	270	1C02	28CB	61.460
10	710	1C05	700	72.200
	710	1C05	71C	21.680
	710	1C05	72N	37.100
	710	1C05	70C	69.880
	710	1C05	72CA	46.020
15	710	1005	76ND2	106.01
	700	1C05	71C	62.240
	700	.1C05	72N	74.850
	700	1C05	70C	17.710
	700	1C05	72CA	96.890
20	700	1C05	76ND2	166.88
	71C	1C05	72N	20.700
	71C	1C05	70C	54.260
	71C	1C05	72CA	38.940
	71C	1C05	76ND2	111.29
25	72N	1C05	70C	61.890
	72N	1C05	72CA	22.050
	72N	1C05	76ND2	95.800
	70C	1C05	72CA	83.310
	70C	1C05	76ND2	149.20
30	72CA	1C05	76ND2	73.940
	70CD2	1C09	70CE2	21.400
	70CD2	1C09	70CG	21.670
	70CE2	1C09	70CG	37.390
	70CE2	1C12	70CD2	21.540
35	200NH2	1014	2080G	65.400
	200NH2	1014	208CB	73.390
	2080G	1014	208CB	19.950
	280D2	1P15	200NH2	73.130
	76ND2	1016	760D1	39.750
40	76ND2	1016	76CG	20.700
	76ND2	1016	250CA	101.94
	76ND2	1016	730G	42.420

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	760D1	1016	7 6CG	19.460
	760D1	1016	250CA	65.930
	760D1	1016	730G	64.870
	76CG	1016	250CA	82.090
5	76CG	1016	730G	49.850
	250CA	1016	730G	95.020
•	200NH2	1017	280D2	79.710
	200NH2	1017	28CG	64.100
	280D2	1017	28CG	18.170
10	280D2	1018	28CG	16.510
	280D2	1018	247NH2	84.690
	280D2	1018	280D1	30.030
	28CG	1018	247NH2	88.990
	28CG	1018	280D1	17.610
15	247NH2	1018	280D1	77.660
	2080G	1P19	250CA	119.39
	2080G	1P19	206NH1	91.290
	2080G	1P19	2470	124.73
	2080G	1P19	206CD	51.730
20	250CA	1P19	206NH1	134.73
	250CA	1P19	2470	54.230
	250CA	1P19	206CD	138.68
	206NH1	1P19	2470	81.340
	206NH1	1P19	206CD	41.710
25	2470	1P19	206CD	95.200
	2080G	1020	250N	151.34
	2080G	1020	250CA	158.25
	2080G	1020	217CE2	77.450
	2080G	1020	208CB	22.490
30	2080G	1020	2470	144.34
	250N	1020	250CA	25.390
	250N	1020	217CE2	75.240
	250N	1020	208CB	131.25
	250N	1020	2470	53.360
35	250CA	1020	217CE2	97.310
	250CA	1020	208CB	136.92
	250CA	1020	2470	57.350
	217CE2	1020	208CB	64.610
	217CE2	1020	2470	103.98
40	208CB	1020	2470	160.34
	206NH1	1021	206CD	63.610
	206NH1	1021	206CZ	23.320
	206NH1	1021	206NE	44.300
				500

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	206NH1	1021	2080G	119.29
	206NH1	1021	200NH2	93.260
	206CD	1021	206CZ	48.080
	206CD	1021	206NE	26.130
5	206CD	1021	2080G	59.000
	206CD	1021	200NH2	72.680
	206CZ	1021	206NE	23.690
	206CZ	1021	2080G	107.07
	206CZ	1021	200NH2	101.44
10	206NE	1021	2080G	84.290
	206NE	1021	200NH2	92.980
	2080G	1021	200NH2	52.780
	250CA	1022	247NE	114.53
	250CA	1022	2470	64.620
15	250CA	1022	247CZ	128.51
	250CA	1022	247CG	95.540
	250CA	1022	250C	23.580
	250CA	1022	247CD	114.32
	250CA	1022	250N	20.550
20	250CA	1022	247NH2	120.77
	250CA	1022	2500	37.250
	247NE	1022	2470	86.700
	247NE	1022	247CZ	21.230
	247NE	1022	247CG	43.200
25	247NE	1022	250C	91.090
	247NE	. 1022	247CD	22,540
	247NE	1022	250N	124.46
	247NE	1022	247NH2	37.560
	247NE	1022	2500	82.000
30	2470	1022	247CZ	107.10
	2470	1022	247CG	44.460
	2470	1022	250C	57.580
	2470	1022	247CD	68.380
	2470	1022	250N	52.860
35	2470	1022	247NH2	123.53
	2470	1022	2500	41.550
	247CZ	1022	247CG	62.780
	247CZ	1022	250C	106.76
	247CZ	1022	247CD	39.430
40	247CZ	1022	250N	143.24
	247CZ	1022		
	247CZ	1022		
	247CG	1022	250C	75.970

	,, ,			
	247CG	1022	247CD	24.070
	247CG	1022	250N	92.820
	247CG	1022	247NH2	80.760
	247CG	1022	2500	58.790
5	250C	1022	247CD	91.780
	250C	1022	250N	37.390
	250C	1022	247NH2	104.02
	250C	1022	2500	18.310
	247CD	1022	250N	115.79
10	247CD	1022	247NH2	58.770
	247CD	1022	2500	77.290
•	250N	1022	247NH2	140.47
	250N	1022	2500	42.510
	247NH2	1022	2500	105.05
15			i.	

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WHAT IS CLAIMED IS:

- 1. A composition comprising a UPPS in crystalline form.
- 2. The composition according to claim 1 wherein said UPPS is a dimer.
- 3. The composition of claim 1 wherein said UPPS is a Streptococcus
- 5 pneumoniae UPPS.

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- 4. The composition according to claim 1 comprising a protein wherein defined by coordinates of Table IA, interatomic distances in Table ΠA, or angles of active site residues listed in Table IIIA, in an essentially pure native form or a homolog thereof.
- 5. A prenyltransferase of claim 4 which is in its native crystalline form.
 - 6. A prenyltransferase according to claims 4 or 5 wherein said prenyltransferase has an active site formed by the amino acids Arg247, Gly250, Arg206, Arg200, Ser208, Tyr217, Asp28, Tyr70, Ile26, Phe72, Asn76, Met27, Ala71 as ligands to IPP.
- 7. A prenyltransferase according to claims 4 or 5 wherein said prenyltransferase has an active site formed by the amino acids Asp28-Arg32, Arg79, Met27, His45, Gly48, Met49, Leu52, Ala71, Tyr70, Leu90, Pro91, Phe94, Phe149 as ligands to FPP.
 - 8. A composition comprising the prenyltransferase of claim 4 in complex with the substrate FPP wherein defined by coordinates of Table IB, interatomic distances in Table IIB, or angles of active site residues listed in Table IIIB.
 - 9. A composition comprising the prenyltransferase of claim 4 in complex with the substrate IPP wherein defined by coordinates of Table IC, interatomic distances in Table IIC, or angles of active site residues listed in Table IIICB.
- 25 10. A heavy atom derivative of a *Streptococcus pneumoniae* UPPS crystal wherein the prenyltransferase comprises a protein having the coordinates listed in Tables IA-IC, IIA-IIC, or IIIA-IIIC.
 - 11. A prenyltransferase according to claim 4 wherein said prenyltransferase is characterized by an $\alpha+\beta$ fold with three layers, $\alpha\beta\alpha$, wherein the β -strands form a six-strand parallel β -sheet and three α -helices pack against one face of the sheet and three to four α -helices located on the opposite face.

12. A composition comprising a *Streptococcus pneumoniae* UPPS in orthorhombic crystalline form having a space group of P2₁2₁2₁.

- 13. The composition according to claim 12 wherein the crystalline form has lattice constants of a = 59.6Å, b = 118.0Å, c = 178.2Å.
- 5 14. The composition according to claim 12 wherein the crystalline form contains two 60 kDa dimers in an asymmetric unit.
 - 15. A composition comprising a *Streptococcus pneumoniae* UPPS in orthorhombic crystalline form having a space group of I2₁2₁2₁.
- 16. A composition comprising a co-crystal of Streptococcus pneumoniae UPPS
 10 in complex with a substrate IPP in orthorhombic crystalline form having a space group selected from the group consisting of P2₁2₁2₁ and I2₁2₁2₁.
 - 17. A composition comprising a co-crystal of *Streptococcus pneumoniae* UPPS in complex with a substrate FPP in monoclinic crystalline form having a space group of P2₁.
- 18. The composition according to claim 17 wherein the crystalline form has lattice constants of a= 58.1 Å, b = 44.6 Å, c = 115.5Å, β = 98.7°.

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- 19. A process for determining a crystal structure form using the structural coordinates of a *Streptococcus pneumoniae* UPPS crystal or portions thereof, to determine a crystal form of a mutant, homologue, or co-complex of a binding pocket or active site by molecular replacement.
- 20. A process of identifying an inhibitor compound capable of binding to and inhibiting the enzymatic activity of a *Streptococcus pneumoniae* UPPS said process comprising:
- a) introducing into a suitable computer program information defining an active site conformation of a UPPS molecule comprising a conformation defined by the coordinates and listed in Table IA, IIA, or IIIA wherein said program displays the three-dimensional structure thereof;
 - b) creating a three dimensional structure of a test compound in said computer program;
- c) displaying and superimposing a model of said test compound on a model of said active site;

d) incorporating said test compound in a biological prenyltransferase activity assay for a prenyltransferase characterized by said active site; and

- e) determining whether said test compound inhibits enzymatic activity in said assay.
- 5 21. A process designing drugs useful for inhibiting UPPS activity using the atomic coordinates of a *Streptococcus pneumoniae* UPPS crystal to computationally evaluate a chemical entity for associating with a active site of a UPPS enzyme.
 - 22. A method of modifying a test UPPS polypeptide comprising:
- a) providing a test UPPS polypeptide sequence having a characteristic that is
 targeted for modification;
 - b) aligning the test UPPS polypeptide sequence with at least one reference UPPS polypeptide sequence for which an X-ray structure is available, wherein the at least one reference UPPS polypeptide sequence has a characteristic that is desired for the test UPPS polypeptide;
- c) building a three-dimensional model for the test UPPS polypeptide using the three-dimensional coordinates of the X-ray structure(s) of the at least one reference UPPS polypeptide and its sequence alignment with the test UPPS polypeptide sequence;
 - d) examining the three-dimensional model of the test UPPS polypeptide for a difference in an amino acid residue as compared to the at least one reference polypeptide, wherein the residues are associated with the desired characteristic; and

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- e) mutating an amino acid residue in the test UPPS polypeptide sequence located at a difference identified in step (d) to a residue associated with the desired characteristic, whereby the test UPPS polypeptide is modified.
- 23. A process of identifying an inhibitor compound capable of inhibiting the enzymatic activity of a *Streptococcus pneumoniae* UPPS according to claim 4, said process comprising:
 - a) carrying out an *in vitro* assay by introducing said compound in a biological prenyltransferase activity assay containing a prenyltransferase according to claim 4; and
 - b) determining whether said test compound inhibits the enzymatic activity of the prenyltransferase in said assay.

24. A product of the process of claim 20 or 23 which is a peptide, peptidomimetic, or synthetic molecule and is useful for inhibiting a metallo-beta lactamase in treatment of bacterial infections in a mammal.

25. A product according to claim 24 wherein said product is a competitive or non-competitive inhibitor of the *Streptococcus pneumoniae* prenyltransferase.

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- 26. A process designing drugs useful for inhibiting Streptococcus pneumoniae UPPS comprising using the atomic coordinates of a Streptococcus pneumoniae UPPS crystal or the atomic coordinates of a Streptococcus pneumoniae UPPS in complex with FPP or IPP to computationally evaluate a chemical entity for associating with the active site of a Streptococcus pneumoniae UPPS.
- 27. The process according to claim 26 comprising the step of using the structure coordinates of *Streptococcus pneumoniae* UPPS to identify an intermediate in a chemical reaction between a prenyltransferase and a compound that is a substrate or inhibitor of said prenyltransferase.
- 28. The process according to claims 26 or 27 wherein said structure coordinates comprise the coordinates listed in Tables IA-IC, IIA-IIC, or IIIA-IIIC.

Figure 1A

Figure 1B

$$01 \\ 05 \\ 09 \\ 012 \\ 017 \\ 0$$

Figure 2A

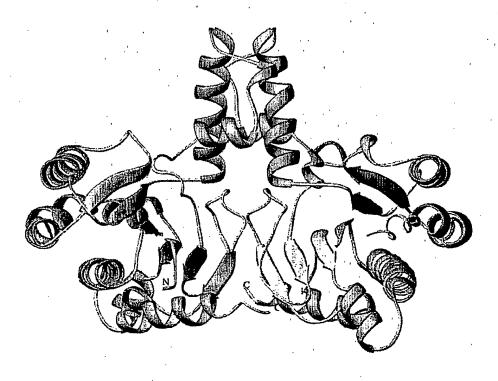


Figure 2B

UPS (S. pneumoniae)

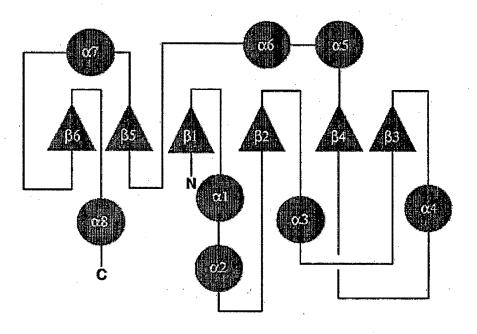


Figure 3A

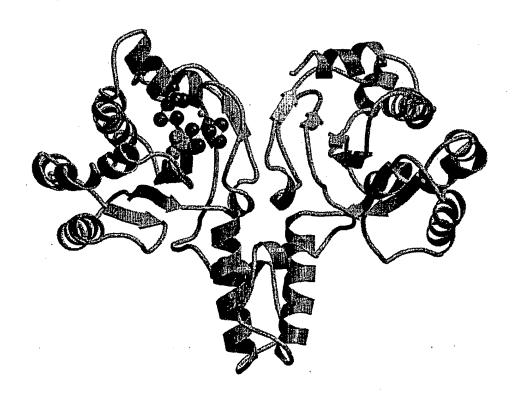


Figure 3B

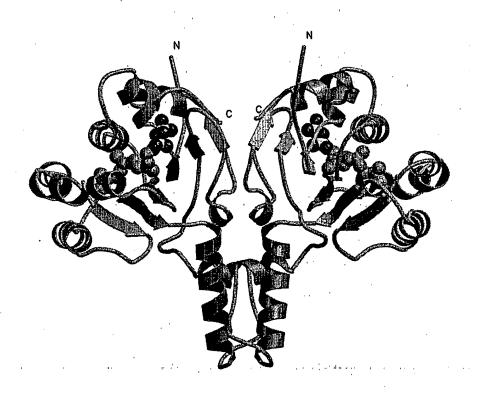


Figure 4A

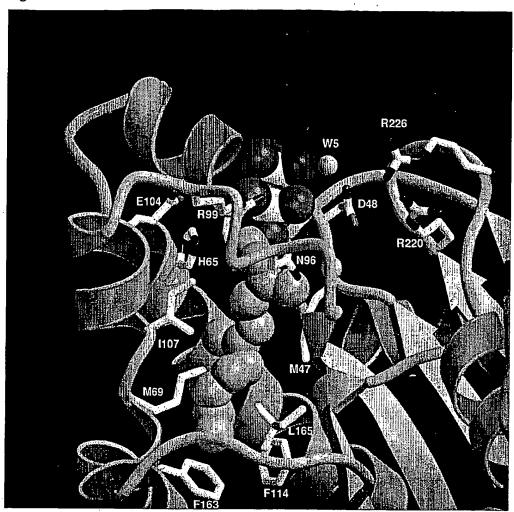
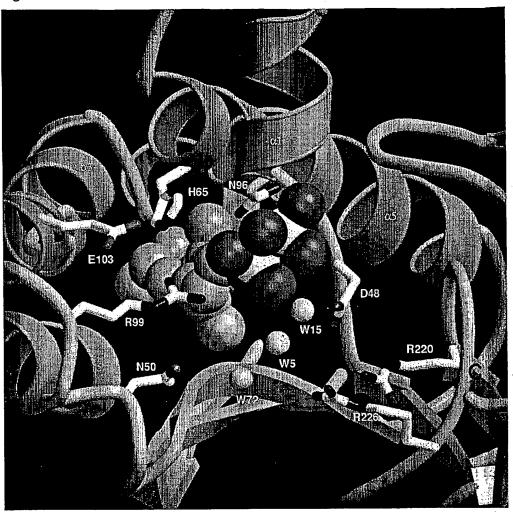
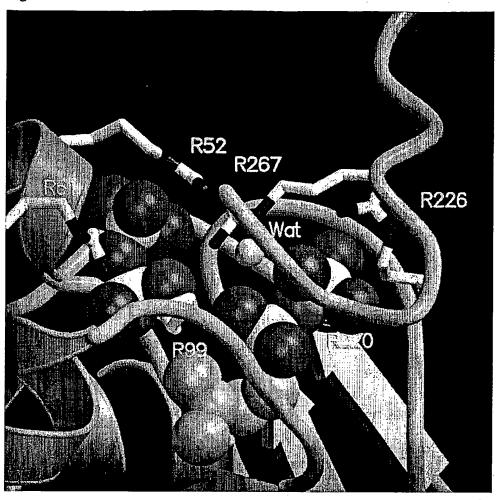


Figure 4B



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Figure 5



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698917InventoryList.txt

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"PCT/US02/38715"

"20 Dec 2002"

"1. DOEO901 Notification of Status of Requirements Under 35 U.S.C. 371"

"2. ISA202 Notification of Receipt of Search Copy"

"3. ISA225 Inv to Furnish Nucleotide and/or Amino Acid Seq Listing Complying with Standard"

"4. RO101 PCT/RO/101 Form Record Copy"

"5. RO101S PCT/RO/101 FORM SEARCH COPY"

"6. RO102N Notification concerning Payment of Prescribed Fees-No R eply"

"7. RO105 Notification of The International Application # and of the Intl. Filing Date"

"8. RO106 Invitation To Correct Defects in The International Application (Incl. Annex ABC)"